

COMPLIANCE WITH THE DATA PROTECTION ACT 1998

In accordance with the Data Protection Act 1998, the personal data provided on this form will be processed by EPSRC, and may be held on computerised database and/or manual files. Further details may be found in the **guidance notes**

EPSRC Reference:

RESEARCH PROPOSAL

You should read the separate notes for guidance and the 'EPSRC Funding Guide' before completing any research proposal. Form Je-SRP1 (EPSRC) must be accompanied by a case for support. EPSRC will reject incomplete research proposals.

1 DETAILS OF PROPOSAL

A. Organisation Where Grant Would Be Held

Organisation: UMIST
 Division or Department: Chemistry

RO Reference: CGOFM

B. Investigators

Please give details of each investigator below. Please provide the details of any additional investigators on a separate sheet using the same format as below.

Details	Principal Investigator (PI)	Co-Investigator 1
Title	Professor	Doctor
Forename(s)	Michael William	Jonathan Robert
Surname	Anderson	Agger
Organisation	UMIST	UMIST
Division or Department	Chemistry	Chemistry
Post will outlast project (Y/N)	Y	Y
% time committed to project	10	25
Other commitments (description and average hours per week)	Directing research projects 12 Writing papers 6 Writing proposals 4 Teaching 2 Departmental administration 4 Research 8	Supervising research students 6 Research 14 Writing papers 4 Writing proposals 2 Teaching 2 Departmental administration 2

Total number of co-investigators (ie. excluding the PI)

4

C. Recognised Researchers

Please give details of each Recognised Researcher below. Please provide the details of any additional Recognised Researchers on a separate sheet using the same format as below.

Details	Recognised Researcher 1	Recognised Researcher 2
Title		
Forename(s)		
Surname		
Organisation		
Division or Department		
% time committed to project		

Total number of Recognised Researchers

0

D. Title of Research Project

(not exceeding 150 characters, including spaces)

Crystal Growth of Open-framework Materials

E. Type of Proposal

Scheme: n/a

Call: n/a

F. Related Proposals

a. If this proposal is related to a previous proposal to EPSRC, please give the previous EPSRC research grant proposal reference number(s) and indicate the type of relationship.

EPSRC Reference Number	How related? (one of Continuation, Follow up to outline proposal, Invited resubmission, Uninvited resubmission)
GR/M10281/01	Follow up

b. If there is more than one organisation submitting a Je-SRP1 (EPSRC) proposal form for this project, please give the number of proposals involved, the lead Research Organisation and the project common reference.

Total Number of Proposals being submitted	Name of Lead RO	Common Reference
2	UMIST	n/a

G. Summary of EPSRC Resources Required for Project

a. Financial resources required

	Total £
Staff	268065
Travel and Subsistence	33720
Consumables	59987
Exceptional Items	34440
Equipment	14837
Large Capital	194450
PCTF	
Sub-total	605499
Indirect Costs	123310
Total	728809

b. Summary of staff effort requested

	Months
Research	54
Technician	7.25
Other	
Project Students	144
Visiting Researchers	
Total	205.25

c. Services

£

H. Start Date and Duration

a. Proposed start date

01/01/04

b. Duration of the grant (months)

36

I. Research Councils / MoD Joint Research Grants Scheme (JGS) If you have received a commitment of support from the Defence Science Technology Laboratory (DSTL), please give the following details:

Percentage funding indicated by DSTL	
DSTL contact (name and address)	
Title/Forename(s)	
Surname	
Address Line 1	
Address Line 2	
Address Line 3	
Town/City	
Administrative Area/County	
Postal Code	
Telephone	
Fax	
E-mail	
DSTL Reference (please ensure that the letter providing this reference is attached with the Case for Support)	

List main objectives of the proposed research in order of priority.

Establish breadth of possible growth mechanisms for open-framework materials.

Establish relationships between structure and growth mechanism.

Study Crystal growth via in-situ atomic force microscopy.

Determine the influence of templates.habit modifiers on growth mechanism.

Identify the units of attachment.

Calculate attachment energies and and crystal surface energies.

Bridge the gap between experiment and theory via simulation of AFM and SEM images.

Exert control over a crystal growth process.

K. Summary

Describe the proposed research using (about 200) words geared to the non-specialist reader.

We propose the most fundamental, ambitious and concerted multi-disciplinary investigation into the understanding crystal growth and rational design of open framework materials yet attempted. We believe the findings from this study will mark a major leap forward into our understanding of crystal growth and our ability to exploit our understanding to produce new materials with unique properties and applications. Extensive studies on the synthesis of porous materials have been carried out. However, the majority of this synthetic work has been aimed primarily at either (i) the discovery of new structures, (ii) modification or improvement of existing materials or (iii) process development to enable such materials to be produced successfully on a large scale. The effort so far on synthesis and crystallisation mechanism has yielded many positive results but also many unanswered questions, for example: (i) the detailed mechanism of nucleation (ii) the identity of growth species and (iii) whether nanocrystal growth occurs by addition or aggregation. This research involves the application of a powerful set of complementary techniques to the study of crystal growth of open-framework materials comprising: atomic force microscopy, high resolution transmission and scanning electron microscopies, in-situ NMR with enhanced data processing, X-ray diffraction and mass spectrometry. A substantially better understanding of the synthesis process is likely to yield important economic benefits, for example, better process control, increased efficiency in reagent usage, improved reproducibility and the capacity to modify or tailor products for specific applications. Perhaps most important of all would be the ability to identify successful synthetic routes to as-yet unknown structures and compositions which have been predicted on theoretical grounds to have beneficial characteristics. Such a step forward to a new level of primary understanding would open the way to innovative applications in chemistry, physics (ordered arrays) and biomaterials.

L. Beneficiaries

Describe who will benefit from the research.

Application-driven technological demands require vastly superior nano-scale control of structure relative to current state-of-the-art. The phenomena of nucleation and crystal growth are inherent to exerting such control. Consequently targeting an improved understanding of these phenomena is vital. The benefits (and predicted impact areas) will include: overcoming crystal size limitations and improving crystal purity (opto-electronics, membrane technology, separations, defense); controlling intergrowth structures and crystal habit (catalysis and water treatment); more cost-effective routes to existing but prohibitively expensive known structures (sensors, batteries, catalysis and biocatalysis).

Ma. Project Studentships

Name/Post Identifier	Start Date	London (Y/N)	Stipend (£)
PhD AFM	01/01/04	N	31500
PhD Microscopy	01/01/04	N	31500
PhD NMR MS XRD	01/01/04	N	31500
PhD Simulation	01/01/04	N	31500
Total			126000

Mb. Visiting Researchers Please provide the details of any additional visiting researchers on a separate sheet in the same format as below.

Details	Visiting Researcher 1	Visiting Researcher 2	Visiting Researcher 3
Title	Professor	Professor	Doctor
Forename(s)	Osamu	Francis	Viveka
Surname	Terasaki	Taulelle	Alfredsson
Home Organisation	University of Stockholm	University of Versailles	Lund University
Division or Department	Structural Chemistry	Institut Lavoisier	Centre for Chemistry & Chemical Eng.
Address Line 1	Arrhenius Laboratory	St Quentin-en-Yvelines	PO Box 124
Address Line 2			
Address Line 3			
Town/City	Stockholm	Versailles	Lund
Administrative Area/County			
Postal Code	S-10691	78035	221 00
Country	Sweden	France	Sweden
Telephone	+46 8 162379	+33 1 39254373	+46 2 228155
Fax	+46 8 163118	+33 3 88607550	+46 2 228155
E-mail	terasaki@struc.su.se	taulelle@chimie.uvsq.fr	viveka.alfredsson@fkem1.lu.se
Post held	Head of Division	Directeur de Recherche	Associate Professor
(a) Will Visiting Researcher be supporting dependants?	N	N	N
(b) What annual salary would host organisation pay staff of the Visiting Researcher's status? (£)	n/a	n/a	n/a
(c) If salary contribution required from EPSRC, state:			
(i) percentage of normal salary being received from any other source	n/a	n/a	n/a
(ii) normal salary if less than given in (b) above (£)	n/a	n/a	n/a

Total number of visiting researchers

3

Mc. Public Communication Training Funds (PCTF)

Do you wish to apply for Public Communication Training Funds? YES NO

N. Travel and Subsistence

Destination and purpose	Total £
(i) Within UK	
4 PhD's to annual BZA meeting	2000
6 staff to one BZA conference	3000
Outside UK - 4 PhD's and 6 staff to IZA meeting	15000
(ii) Outside UK	
6x Sweden-Manchester with 4 nights accomodation for Terasaki and Alfrdsson (6 monthly meetings)	7920
6x France-Manchester with 4 nights accomodation for Taulelle (6 monthly meetings)	3360
2x Sweden Manchester with 4 nights accomodation for PhD microscopy (2 of the 6 monthly meetings)	1320
2x France Manchester with 4 nights accomodation for PhD NMR MS XRD (2 of the 6 monthly meetings)	1120
Total £	33720

O. Consumables

Description	Total £
5x 20 silicon nitride probes for AFM	717
2x 70 tapping mode etched silicon probes for AFM	2073
10% Running costs for NMR spectrometer (1560L of liq. N2 and 186L of liq. He)	1097
Access charges for HREM (144 days @ £71 per day)	10224
Access charges for SEM (288 2 hour slots @ £59 per 12 hours)	2832
Access charges for NMR spectrometer (144 days @ £71 per day)	10224
Access charges for Mass spectrometer (144 hours @ £30 per hour)	4320
Stationary for PhD (simulation)	1500
Chemicals for synthesis @£2000 pa per experimentalist	27000
Total £	59987

P. Exceptional Items

Description	Total £
Tuition fees for 4 PhD students @ £8610 per student	34440
Total £	34440

Description	Country of Manufacture	Delivery Date	Basic price £	Import duty £	VAT £	Total £
EMITECH Turbo Cr Sputter Coater + pump 2 PC computers	UK	01/01/04	9983		1763	11837
	UK	01/01/04	2554		446	3000
					Total £	14837

R. Large Capital (single items £100,000 and over)

Description	Country of Manufacture	Delivery Date	Basic price £	Import duty £	VAT £	Total £
Veeco AFM with heated stage and acoustic/vibration isolation table.	USA	01/01/04	165489		28961	194450
					Total £	194450

Sa. Services

Service	Instrument(s)	Units	Cost £
		Total	

T. Other Support

Give details of any support sought or received from any source for this or related research in the past three years (minimum £10,000)

Awarding Organisation	Awarding Organisation's Reference	Title of project	Start Date	End Date	Amount Sought/ Awarded (£)	Date Decision Expected/ Made

U. Project Partners

Please give details of partners in the project and their contributions to the research. These contributions should be in addition to resources identified above. If there are more than two partner organisations, please provide details on a separate sheet using the same format as below.

Details	Partner 1	Partner 2		
Name of partner organisation				
Division/Department				
Address Line 1				
Address Line 2				
Address Line 3				
Town/City				
Administrative Area/County				
Postal Code				
Country				
Organisation Type				
Main Standard Industrial Code				
Number of Employees				
Annual Turnover (£)				
Title/Forename(s) of Contact				
Surname of Contact				
Contact's Address (if different from organisation address)				
Address Line 1				
Address Line 2				
Address Line 3				
Town/City				
Administrative				
Postal Code				
Country				
Telephone				
Fax				
E-mail				
Direct contribution to project	Description	Value £	Description	Value £
a. cash				
b. equipment/materials				
c. secondment of staff				
d. other				
Sub-Total				
Indirect contribution to project				
a. use of facilities/equipment				
b. staff time				
c. other				
Sub-Total				
Total Contribution				
Total Value (including contributions from additional project partners)				

Total number of project partners

2 OTHER INFORMATION

Information in this section will be used for administrative purposes and will NOT be circulated to referees or panels.

A. Nominated Referees

Please give details of 3 referees whom the EPSRC may approach for assessment of this research proposal.

Details	Referee 1	Referee 2
Title	Professor	Professor
Forename(s)	Anthony	Jacek
Surname	Cheetham	Klinowski
Organisation	University of California Santa Barbara	University of Cambridge
Division or Department	Materials Research Laboratory	Department of Chemistry
Address Line 1	Materials Research Laboratory	Lensfield Road
Address Line 2	University of California	
Address Line 3		
Town/City	Santa Barbara	Cambridge
Administrative Area	California	Cambridgeshire
Postal Code	93106	CB2 1EW
Country	USA	United Kingdom
Telephone	+1 805 893 8767	+44 (0)1223 336514
Fax	+1 805 893 8797	+44 (0)1223 336362
E-mail	cheetham@mrl.ucsb.edu	jk18@cam.ac.uk

Details	Referee 3
Title	Doctor
Forename(s)	Paul
Surname	Wright
Organisation	University of St Andrews
Division or Department	Chemistry
Address Line 1	Purdie building
Address Line 2	
Address Line 3	
Town/City	St Andrews
Administrative Area	Fyfe
Postal Code	KY16 9ST
Country	United Kingdom
Telephone	+44 (0)1334 463793
Fax	+44 (0)1334 463808
Email	paw2@st-and.ac.uk

B. Declaration

In submitting this research proposal, I confirm on behalf of the Administrative Authority of [Name of Submitting Organisation] that:

- a. we have read and understood the requirements in the EPSRC Funding Guide and have checked that the proposal complies with these
- b. if a grant is offered we will accept the terms and conditions applied by EPSRC
- c. we have not entered into any obligations which may conflict with the EPSRC terms and conditions

Name in BLOCK CAPITALS: Colin Cooper**Position: Head RGCA****Signature:****Date:**

	Name in BLOCK CAPITALS	Signature	Date
Principal Investigator	Michael Anderson		30/06/03
Co-Investigators	Jonathan Agger Colin Cundy Simon Gaskell Martin Attfield		30/06/03
Recognised Researchers			
Head of Department	Bob Munn		30/06/03

3. PERSONAL INFORMATION

Information in this section will be used for administrative and statistical purposes and will NOT be circulated to referees or panels.

B. Investigators Please give details of each investigator below. Please provide the details of any additional investigators on a separate sheet using the same format as below.

Details	Principal Investigator	Co-Investigator 1
PID		
Suffix (eg FRS)	BSc PhD FRSC CChem	BSc PhD MRSC CChem
Preferred form of name	Mike	Jonathan
Telephone	0161 200 4517	0161 200 4527
Fax	0161 200 4559	0161 200 4559
E-mail	m.anderson@umist.ac.uk	j.agger@umist.ac.uk
Date of Birth	28/01/60	21/03/70
Sex	Male	Male
Ethnic Origin	White - British	White - British
Disability (Y/N, details of	N	N
Current Post	Professor of Materials Chemistry	EPSRC Advanced Research Fellow
Current Post Start Date	01/10/98	01/10/99
Sector	Higher Education Institution	Higher Education Institution
Function	Academic	Fellow
Expertise (This information may be used to help identify expertise in a given area and to select potential referees).	Experimental and theoretical NMR studies of heterogeneous microporous catalysts; structural studies of mesoporous materials; atomic force microscopy and electron microscopy studies of crystallisation mechanisms; synthesis and applications of novel microporous materials.	Solid-state NMR and atomic force microscopy studies of crystal growth in microporous materials. The application of computer simulation to the interpretation of measured topography and morphology.

C. Recognised Researchers Please give details of each Recognised Researcher below. Please provide the details of any additional Recognised Researchers on a separate sheet using the same format as below.

Details	Recognised Researcher 1	Recognised Researcher 2
PID		
Suffix (eg FRS)		
Preferred form of name		
Telephone		
Fax		
E-mail		
Date of Birth		
Sex		
Ethnic Origin		
Disability (Y/N, details of		
Current Post		
Current Post Start Date		
Sector		
Function		

... be used to help identify expertise in a given area and to select potential referees).

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EPSRC Reference:

RESEARCH PROPOSAL

You should read the separate notes for guidance and the 'EPSRC Funding Guide' before completing any research proposal. Form Je-SRP1 (EPSRC) must be accompanied by a case for support. EPSRC will reject incomplete research proposals.

1 DETAILS OF PROPOSAL

A. Organisation Where Grant Would Be Held

Organisation: Royal Institution of Great Britain

RO Reference: CGFS

Division or Department: Davy Faraday Laboratory

B. Investigators

Please give details of each investigator below. Please provide the details of any additional investigators on a separate sheet using the same format as below.

Details	Principal Investigator (PI)	Co-Investigator 1
Title	Doctor	Professor
Forename(s)	Ben	Stephen C
Surname	Slater	Parker
Organisation	Royal Institution	University of Bath
Division or Department	Davy Faraday Laboratory	Chemistry
Post will outlast project (Y/N)	Y	Y
% time committed to project	10	10
Other commitments (description and average hours per week)	Directing research projects 12 Writing papers 6 Writing proposals 4 Teaching 0 Departmental administration 8 Research 8	Directing research projects 12 Writing papers 6 Writing proposals 4 Teaching 2 Departmental administration 4 Research 8

Total number of co-investigators (ie. excluding the PI)

2

C. Recognised Researchers

Please give details of each Recognised Researcher below. Please provide the details of any additional Recognised Researchers on a separate sheet using the same format as below.

Details	Recognised Researcher 1	Recognised Researcher 2
Title		
Forename(s)		
Surname		
Organisation		
Division or Department		
% time committed to project		

Total number of Recognised Researchers

0

D. Title of Research Project

(not exceeding 150 characters, including spaces)

Crystal Growth of Open-framework Materials

E. Type of Proposal

Scheme: n/a

Call: n/a

F. Related Proposals

a. If this proposal is related to a previous proposal to EPSRC, please give the previous EPSRC research grant proposal reference number(s) and indicate the type of relationship.

EPSRC Reference Number	How related? (one of Continuation, Follow up to outline proposal, Invited resubmission, Uninvited resubmission)
GR/M10281/01	Follow up

b. If there is more than one organisation submitting a Je-SRP1 (EPSRC) proposal form for this project, please give the number of proposals involved, the lead Research Organisation and the project common reference.

Total Number of Proposals being submitted	Name of Lead RO	Common Reference
2	UMIST	n/a

G. Summary of EPSRC Resources Required for Project

a. Financial resources required

	Total £
Staff	112500
Travel and Subsistence	18900
Consumables	21970
Exceptional Items	25830
Equipment	9909
Large Capital	
PCTF	
Sub-total	189109
Indirect Costs	51750
Total	240859

b. Summary of staff effort requested

	Months
Research	
Technician	0
Other	
Project Students	108
Visiting Researchers	
Total	108

c. Services

£

H. Start Date and Duration

a. Proposed start date

01/01/04

b. Duration of the grant (months)

36

I. Research Councils / MoD Joint Research Grants Scheme (JGS) If you have received a commitment of support from the Defence Science Technology Laboratory (DSTL), please give the following details:

Percentage funding indicated by DSTL	
DSTL contact (name and address)	
Title/Forename(s)	
Surname	
Address Line 1	
Address Line 2	
Address Line 3	
Town/City	
Administrative Area/County	
Postal Code	
Telephone	
Fax	
E-mail	
DSTL Reference (please ensure that the letter providing this reference is attached with the Case for Support)	

List main objectives of the proposed research in order of priority.

- Establish breadth of possible growth mechanisms for open-framework materials.
- Establish relationships between structure and growth mechanism.
- Study Crystal growth via in-situ atomic force microscopy.
- Determine the influence of templates/habit modifiers on growth mechanism.
- Identify the units of attachment.
- Calculate attachment energies and crystal surface energies.
- Bridge the gap between experiment and theory via simulation of AFM and SEM images.
- Exert control over a crystal growth process.

K. Summary

Describe the proposed research using (about 200) words geared to the non-specialist reader.

We propose the most fundamental, ambitious and concerted multi-disciplinary investigation into the understanding crystal growth and rational design of open framework materials yet attempted. We believe the findings from this study will mark a major leap forward into our understanding of crystal growth and our ability to exploit our understanding to produce new materials with unique properties and applications. Extensive studies on the synthesis of porous materials have been carried out. However, the majority of this synthetic work has been aimed primarily at either (i) the discovery of new structures, (ii) modification or improvement of existing materials or (iii) process development to enable such materials to be produced successfully on a large scale. The effort so far on synthesis and crystallisation mechanism has yielded many positive results but also many unanswered questions, for example: (i) the detailed mechanism of nucleation (ii) the identity of growth species and (iii) whether nanocrystal growth occurs by addition or aggregation. This research involves the application of a powerful set of complimentary techniques to the study of crystal growth of open-framework materials comprising: atomic force microscopy, high resolution transmission and scanning electron microscopies, in-situ NMR with enhanced data processing, X-ray diffraction and mass spectrometry. An improved understanding of the synthesis process is likely to yield important economic benefits, for example, better process control, increased efficiency in reagent usage, improved reproducibility and the capacity to modify or tailor products for specific applications. Perhaps most important of all would be the ability to identify successful synthetic routes to as-yet unknown structures and compositions which have been predicted on theoretical grounds to have beneficial characteristics. Such a step forward to a new level of primary understanding would open the way to innovative applications in chemistry, physics (ordered arrays) and biomaterials.

L. Beneficiaries

Describe who will benefit from the research.

Application-driven technological demands require vastly superior nano-scale control of structure relative to current state-of-the-art. The phenomena of nucleation and crystal growth are inherent to exerting such control. Consequently targeting an improved understanding of these phenomena is vital. The benefits (and predicted impact areas) will include: overcoming crystal size limitations and improving crystal purity (opto-electronics, membrane technology, separations, defense); controlling intergrowth structures and crystal habit (catalysis and water treatment); more cost-effective routes to existing but prohibitively expensive known structures (sensors, batteries, catalysis and biocatalysis).

Ma. Project Studentships

Name/Post Identifier	Start Date	London (Y/N)	Stipend (£)
PhD Atomistic calculation * 2	01/01/04	Y	75000
PhD Atomistic calculation	01/01/04	N	31500
Total			112500

Mb. Visiting Researchers Please provide the details of any additional visiting researchers on a separate sheet in the same format as below.

Details	Visiting Researcher 1	Visiting Researcher 2	Visiting Researcher 3
Title	Professor	Professor	Doctor
Forename(s)	Osamu	Francis	Viveka
Surname	Terasaki	Taulelle	Alfredsson
Home Organisation	University of Stockholm	University of Versailles	Lund University
Division or Department	Structural Chemistry	Institut Lavoisier	Centre for Chemistry & Chemical Eng.
Address Line 1	Arrhenius Laboratory	St Quentin-en-Yvelines	PO Box 124
Address Line 2			
Address Line 3			
Town/City	Stockholm	Versailles	Lund
Administrative Area/County			
Postal Code	S-10691	78035	221 00
Country	Sweden	France	Sweden
Telephone	+46 8 162379	+33 1 39254373	+46 2 228155
Fax	+46 8 163118	+33 3 88607550	+46 2 228155
E-mail	terasaki@struc.su.se	taulelle@chimie.uvsq.fr	viveka.alfredsson@fkem1.lu.se
Post held	Head of Division	Directeur de Recherche	Associate Professor
(a) Will Visiting Researcher be supporting dependants?	N	N	N
(b) What annual salary would host organisation pay staff of the Visiting Researcher's status? (£)	n/a	n/a	n/a
(c) If salary contribution required from EPSRC, state:			
(i) percentage of normal salary being received from any other source	n/a	n/a	n/a
(ii) normal salary if less than given in (b) above (£)	n/a	n/a	n/a

Total number of visiting researchers

3

Mc. Public Communication Training Funds (PCTF)

Do you wish to apply for Public Communication Training Funds? YES NO

N. Travel and Subsistence

Destination and purpose	Total £
(i) Within UK	
6x London,Bath/Manchester with 2 nights accomodation for Slater, Lewis and PhD (6 monthly meetings)	5100
Meeting costs for 1 British Zeolites Association meeting per PhD student, per year * 3	1800
Meeting costs for 1 British Zeolites Association meeting per investigator * 3	1500
(ii) Outside UK	
1 international meeting ACS or MRS for each PhD student in the course of their PhD (including flights, meeting fees, accommodation) * 3	4500
1 international meeting ACS or MRS for each investigator * 3	6000
Total £	18900

O. Consumables

Description	Total £
General Computing Consumables, including additional hardware for data storage, ie hard disks, + high resolution printer, cpu upgrade at 1500pa	4500
Accelrys software licenses	
Materials Studio	1569
CASTEP interface	1256
Consumables and licenses are essential for each investigator, hence the total reflects the costs for the three institutions	
Total £	21975

P. Exceptional Items

Description	Total £
Tuition fees for three PhD students @ £8610	25830
Total £	25830

Description	Country of Manufacture	Delivery Date	Basic price £	Import duty £	VAT £	Total £
High performance computer workstation 1 per PhD researcher Dell precision workstation 650 Dual Athlon Intel Xeon 3Ghz 2Gb RAM, 120GB Hard Drive, 21" Monitor	UK	01/01/04	2811		492	3303
					Total £	9909

R. Large Capital (single items £100,000 and over)

Description	Country of Manufacture	Delivery Date	Basic price £	Import duty £	VAT £	Total £
					Total £	

Sa. Services

Service	Instrument(s)	Units	Cost £
		Total	

T. Other Support

Give details of any support sought or received from any source for this or related research in the past three years (minimum £10,000)

Awarding Organisation	Awarding Organisation's Reference	Title of project	Start Date	End Date	Amount Sought/ Awarded (£)	Date Decision Expected/ Made

J. Project Partners

Please give details of partners in the project and their contributions to the research. These contributions should be in addition to resources identified above. If there are more than two partner organisations, please provide details on a separate sheet using the same format as below.

Details	Partner 1		Partner 2	
Name of partner organisation				
Division/Department				
Address Line 1				
Address Line 2				
Address Line 3				
Town/City				
Administrative Area/County				
Postal Code				
Country				
Organisation Type				
Main Standard Industrial Code				
Number of Employees				
Annual Turnover (£)				
Title/Forename(s) of Contact				
Surname of Contact				
Contact's Address (if different from organisation address)				
Address Line 1				
Address Line 2				
Address Line 3				
Town/City				
Administrative				
Postal Code				
Country				
Telephone				
Fax				
E-mail				
Direct contribution to project	Description	Value £	Description	Value £
a. cash				
b. equipment/materials				
c. secondment of staff				
d. other				
Sub-Total				
Indirect contribution to project				
a. use of facilities/equipment				
b. staff time				
c. other				
Sub-Total				
Total Contribution				
Total Value (including contributions from additional project partners)				

Total number of project partners

2 OTHER INFORMATION

Information in this section will be used for administrative purposes and will NOT be circulated to referees or panels.

A. Nominated Referees

Please give details of 3 referees whom the EPSRC may approach for assessment of this research proposal.

Details	Referee 1	Referee 2
Title	Reader	Reader
Forename(s)	Julian	Neil
Surname	Gale	Allan
Organisation	Imperial College	Bristol University
Division or Department	Chemistry	Chemistry
Address Line 1	South Kensington	
Address Line 2		
Address Line 3		
Town/City	London	Bristol
Administrative Area		
Postal Code	SW7 2AY	BS8 1TS
Country	UK	UK
Telephone		
Fax		
E-mail	j.gale@ri.ac.uk	n.l.allan@bristol.ac.uk

Details	Referee 3
Title	Professor
Forename(s)	Russell
Surname	Morris
Organisation	University of St. Andrews
Division or Department	School of Chemistry
Address Line 1	North Haugh
Address Line 2	
Address Line 3	
Town/City	St Andrews
Administrative Area	Fife
Postal Code	KY16 9ST
Country	
Telephone	01334 463818
Fax	01334 463808
Email	rem1@st-and.ac.uk

3. PERSONAL INFORMATION

Information in this section will be used for administrative and statistical purposes and will NOT be circulated to referees or panels.

B. Investigators Please give details of each investigator below. Please provide the details of any additional investigators on a separate sheet using the same format as below.

Details	Principal Investigator	Co-Investigator 1
PID		
Suffix (eg FRS)	BSc PhD	BSc PhD MRSC CChem
Preferred form of name	Ben	Steve
Telephone	+44 (0)20 7670 2954	+44 (0)1225 386505
Fax	+44 (0)20 7629 3569	+44 (0)1225 386231
E-mail	ben@ri.ac.uk	s.c.parker@bath.ac.uk
Date of Birth	18/03/1970	17/09/1957
Sex	Male	Male
Ethnic Origin	White - British	White - British
Disability (Y/N, details of	N	N
Current Post	Senior Research Fellow/Asst. Director	Professor
Current Post Start Date	1/10/1999	1/10/1984
Sector	Higher Education Institution	Higher Education Institution
Function	Academic	Academic
Expertise (This information may be used to help identify expertise in a given area and to select potential referees).	Atomistic, molecular and solid state simulation techniques including electronic structure methods, energy minimisation, molecular dynamics and Monte Carlo. Zeolite and complex minerals structural chemistry Predicting surface structure and crystal morphology modelling. High performance computing Code development (Fortran/C)	Atomistic modelling techniques including free-energy minimisation, electronic structure methods, Monte Carlo and molecular dynamics. Expertise in crystal growth modelling Software development in Fortran High performance computing Mineral chemistry

C. Recognised Researchers Please give details of each Recognised Researcher below. Please provide the details of any additional Recognised Researchers on a separate sheet using the same format as below.

Details	Recognised Researcher 1	Recognised Researcher 2
PID		
Suffix (eg FRS)		
Preferred form of name		
Telephone		
Fax		
E-mail		
Date of Birth		
Sex		
Ethnic Origin		
Disability (Y/N, details of		
Current Post		
Current Post Start Date		
Sector		
Function		

Expertise (the information may be used to help identify expertise in a given area and to select potential referees).

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SUMMARY OF RESULTS AND CONCLUSIONS OF RECENT WORK

Anderson has substantial experience over 20 years in the study of microporous materials publishing work in over 150 papers. He received the Royal Society of Chemistry Barrer Award in 1993 for distinguished work on zeolites and was recently Chairman of the British Zeolite Association. His specific interests include: experimental and theoretical NMR studies of heterogeneous microporous catalysts; structural studies of mesoporous materials; atomic force microscopy and electron microscopy studies of crystallisation mechanisms; synthesis and applications of novel microporous materials. It is these last two areas which are pertinent to the current application. Anderson is currently Director of the UMIST Centre for Microporous Materials (UCMM), <http://www.ch.umist.ac.uk/cmm>, which is housed in a recently refurbished suite of laboratories that is extremely well equipped for the study of porous materials. The only major item of equipment which we request for this work is a special atomic force microscope which is integrated with an optical microscope for manipulating and observing micron-sized crystals.

Agger, Attfield and Cundy are all Associate Directors at the UCMM with collective experience respectively in crystal growth by AFM, crystallography of microporous materials, synthetic methods. Agger is an Advanced EPSRC Fellow and Attfield is a Royal Society University Research Fellow. Cundy worked at ICI for 20 years concentrating on inorganic and mineralogical chemistry and specialising in clays and zeolites. He joined the staff at UCMM in 1994.

In 1996 Anderson and Agger reported the first ever study of the crystallisation of a synthetic zeolite by atomic force microscopy, concluding that: growth of zeolite Y occurred *via* layer-upon layer deposition; the area of each layer increased linearly with time; layer structure, but not specific termination, could be determined.^[1] In 1998 they reported similarities in the growth of zeolite A and proposed a complete mechanism to explain the observed surface topography, based on the likelihood of nutrient attachment being related to structural connectivity.^[2,3] This was subsequently corroborated by the creation of a computer simulation of the growth which revealed for the first time probabilities for fundamental growth processes.^[4] A reviewer to the work first published in *Angew. Chem. Int. Ed.* commented, "One of the very best papers I ever read on the simulation of growth. I consider this paper as *very important* and am really enthusiastic". An AFM study of the multiple facets of SSZ-42 discussed the specific role of organic structure directing agents.^[5] The AFM work has been reviewed and put into the context of other studies.^[6,7] A further simulation of the inherently more complex zeolite Y structure^[8] in conjunction with an AFM study by Singh *et al.* on ZnPO-X^[9] crystals led to conclusions on the fundamental growth unit of FAU type structures. In 2003, Agger, Anderson and Cundy published a detailed study of the crystal growth of silicalite.^[10] The simplest observed growth of this material strongly resembles growth of zeolites A and Y. Layer spreading rates appear identical on different crystallographic faces and it is the much slower, rate of nucleation of successive layers that governs the overall growth rate of a face and determines the well known linear crystal growth highlighted by Cundy *et al.* in 1993.^[11] However, silicalite growth is susceptible to defect incorporation – the proposed mechanism for such inclusion has important ramifications on crystal intergrowths. Agger and Anderson recently published an AFM study of a metal substituted aluminophosphate material^[12] and the work suggests an interesting link between chemical composition, structure and crystal morphology.

Cundy has great experience of zeolite synthesis and has recently published a comprehensive review.^[13] He and Plaisted have performed extensive studies on the synthesis of zeolite ZSM-5 under very carefully controlled conditions^[14-16] and these samples will be used in part of the proposed work.

Gaskell, who runs one of the top mass spectrometry facilities in the UK and will be responsible for some of the solution speciation studies, has over 200 peer reviewed papers concerning the development and application of the technique.

Slater, Parker and Lewis are leading exponents of atomistic computer simulation methods and have cumulatively published in excess of 250 papers over 50 of which are focused upon modelling zeolite crystal bulk structure, surface structure and processes within microporous materials. Their work concentrates heavily upon understanding the phenomenon of crystal growth within microporous materials and other complex minerals.

Slater is a senior research fellow and assistant director at the Davy Faraday Research Laboratory and has substantial experience of a wide range of classical and first-principles methods in atomistic computer simulation. He has authored over 30 papers concerning materials as diverse as molecular crystals, metal-oxides and microporous materials, with an emphasis on *surface* structure and *surface* processes. Recently, he has focused on developing predictive methods (including extensions to the widely used MARVIN surface simulation code) and approaches to determine the surface structure of zeolites.^[17,18]

Parker joined the University of Bath in 1984 and was appointed a full professor in 1998. He has published 160 scientific papers and in recent years there have been two main themes, firstly, developing and applying atomistic simulation techniques to model the thermodynamics and phase transitions in solids and secondly, modelling the surface properties of oxides and minerals^[23-26]. Successes have included predicting the negative thermal expansion of many zeolites^[23-25], evaluating the interaction of water with oxide surfaces^[26-30] and calculating the competitive adsorption of inorganic and organics^[31-33].

Lewis is a senior lecturer at UCL and has an extensive body of work in the field of modelling microporous solids with over 50 publications. He has been awarded the RSC Meldola medal and the MSI Academic prize. The overall goal has been to establish programmes of fundamental studies of zeolite synthesis, whilst also developing methodologies that facilitate the discovery of new materials; for example, the *de novo* design of templating agents.^[34] Recently, he has focussed on the modelling of hydrated zeolites, elucidating mechanisms of structure ordering and dehydration processes.

To date the UK is world leading in efforts to understand crystallisation mechanisms in this very important class of material. However, interest in the field is steadily growing as atomic force microscopes become more prevalent in academic institutions, particularly in the US and in Japan. Consolidating the pre-eminent position of the UK necessitates a wide range of skills and knowledge of applying those skills to the highly multi-disciplinary problem of crystal growth in open-framework materials. It is thus impossible to work solely with scientists from the UK. Consequently, the team involves some of the world's experts in a manner which will both allow the team to achieve its aims but also to import technology and future skills into the UK. In this regard we draw upon the expertise of: Professor Osamu Terasaki – the world's leading expert in the application of high-resolution electron microscopy (HREM) to the study of porous framework materials with particular interest in the application of such methods to crystal growth; Professor Francis Taulelle – one of the world's leading experts in the application of NMR methods to the study of crystallisation pathways in porous materials; Dr Viveka Alfredsson – who also has considerable expertise in the application of HREM to the study of porous materials. The UMIST group have a long-standing collaboration with Professor Terasaki who has also published joint papers with the group at the Royal Institution(RI). The groups at the RI, UCL and Bath have ongoing collaborations between their groups in addition to those with Anderson, Agger and Terasaki. Dr Alfredsson spent a productive year working at UMIST as a PDRA and Professor Taulelle has visited Manchester to present a plenary lecture at one of our symposium series.

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CRYSTAL GROWTH IN OPEN FRAMEWORK INORGANIC MATERIALS

BACKGROUND

This proposal concerns crystal-growth mechanisms in open-framework materials. Our approach is multi-disciplinary involving the world's leading experts in the study of a generic problem. To appreciate its importance and timeliness and why such substantial investment should be made by EPSRC it is necessary to understand the history of the subject, the role of UK science therein and the potential wide-ranging benefits.

History

Solid-state materials fall into a number of different categories differentiated either in terms of chemistry (*i.e.* structure, bonding, crystallography, composition etc.) or in terms of properties (*i.e.* applications or potential applications). In chemical terms one very large class of materials with many interesting and important properties is that of open-framework structures. What sets this class of materials apart from other materials is the potential (often unrealised) for highly ordered porosity whereby the entire solid material can be tangibly accessed by guest molecules. Such a highly desirable property - for many applications from catalysis to separations to sensors - is unique to this class of material. The archetypal material usually chosen to typify this class is the zeolite (crystalline aluminosilicate), however, a wide variety of framework compositions now exist including both fully inorganic and inorganic/organic hybrid networks.

How crystals nucleate and grow is a problem that has challenged scientists for many years.^[35-37] How order is created from disorder, the driving forces involved, the quest for crystalline perfection. In many ways nucleation and crystal growth should not be considered as separate phenomena, however, for practical reasons it is useful to do so. The techniques at our disposal to follow the nucleation and crystal growth stages are substantially different and therefore there is often a visible seam between our perception of the two processes. In terms of crystal growth the advent of scanning probe microscopies^[38] (SPM) and in particular atomic force microscopy^[39] (AFM) has permitted the detailed observation of nanometer-sized events at crystal surfaces. This is often possible under *in situ* crystal-growth conditions as the technique can be operated to observe surfaces under solution. Real-time images of growing crystals have revealed terrace growth, spiral growth, the inclusion of defects and the occlusion of foreign particles in a wide variety of growth studies.^[40] The effect of altering the growth medium on individual growth processes can be studied, for instance by adding proteins during the growth of abalone. Enhanced or retarded growth rates which result in altered morphology can be observed.^[41] By measuring real-time micrographs at a range of temperatures the free-energy for individual growth processes can be determined. To date most of these crystal growth studies have been on dense phase ionic crystals, such as calcite, or molecular crystals, such as proteins and viruses. There has been a modest amount of work performed on open-framework crystals such as zeolites and zeotypes of which we have been at the forefront.^[1-3,5,9,10,42-44] The reason for this is two-fold: first, often the most interesting open-framework structures can only be crystallised as micron-sized crystals, making observation by AFM a little more challenging; second, there has been a recent emphasis within the community on making new materials rather than on understanding formation. In our view, this is an oversight which is clear by the vast amount of new information forthcoming on understanding crystal growth in macromolecular systems which is helping address problems such as: overcoming crystal size limitations; improving crystal purity; controlling intergrowth structures, controlling crystal habit. In open-framework materials a better understanding of the crystal growth processes will lead to new methodologies to control similarly important crystal features. But furthermore it could lead to both new structures and also more cost-effective routes to existing but prohibitively expensive known structures.

The role of UK scientists

The UK has been at the forefront of utilising atomic force microscopy in the study of fundamental crystal growth processes in framework materials through work at UMIST (Anderson, Agger). Also the teams at the Royal Institution (Slater), UCL (Lewis) and at Bath University (Parker) are leading in the use of modelling techniques to study energetics at the surfaces of framework materials. Furthermore, there is a wide literature concerning crystal growth of framework materials *via* conventional means utilising optical microscopy and particle-size counting in highly controlled environments. Cundy, at UMIST, worked in this area at ICI for some 20 years and has an extensive knowledge of the lessons learnt from this wealth of data enabling new results to be considered in the light of previous knowledge. Although AFM and theoretical studies are two of the most important recent routes to probe crystal growth pathways they must be supplemented by other techniques, in particular: high-resolution electron microscopy; NMR; diffraction; more recently mass spectrometry. The UK has not been at the forefront in this regard. Professor Osamu Terasaki at Stockholm University is the world's leading expert in the study of surface structure in framework materials by electron microscopy. Both the UMIST and RI groups have long standing collaborations with Professor Terasaki. Similarly, in terms of speciation during crystal growth monitored by NMR methods, Professor Francis Taulelle from Strasbourg is currently the world's leading expert. Consequently, the purpose of this proposal is both to bring to bear the strength of our combined expertise but also to effect a knowledge transfer from these leading groups to the UK for the future. This should enable the UK to consolidate its pre-eminence in the area of crystal growth of open-framework materials. Finally, one of the most exciting new developments is the potential of mass spectrometry to monitor speciation *in situ* during crystal growth. This has been demonstrated by Schüth in Mülheim^[45]. At UMIST we are particularly

well equipped through the Michael Barber Centre for Mass Spectrometry (Gaskell) to integrate such measurements into these studies.

Wide-ranging benefits

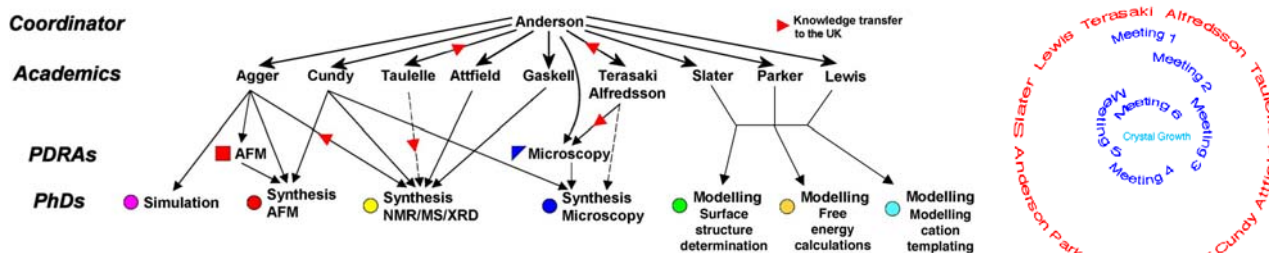
The far-reaching consequences of this work can be illustrated with a prediction. Many open-framework inorganic materials are synthesised using expensive organic templates. The full role of these templates is at present unclear, however, if the primary role during crystal growth is to promote surface nucleation, then the concentration might be reduced to a level where nucleation still occurs and a less expensive space filler may be employed to continue growth of new crystalline layers. This is a single predictive example - but one might also envisage novel controlled intergrowth structures; defect free structures; controlled crystal habit; crystals embedded within crystals; massive crystals; single crystal films; epitaxial growth of materials with complementary properties. Such complexity eludes the community at present because a far better understanding of the crystal growth process is required.

PROGRAMME AND METHODOLOGY

The overall aim of the project is to substantially improve our understanding of crystallisation processes in open-framework materials, bridging the gap between the different, yet complementary chemistries of the solution and the growing solid surface. A close synergy will be developed between the experimental work and atomistic calculations.

There are three things which must be coupled for the success of the project: (i) the major problems to be addressed; (ii) the techniques at our disposal; (iii) the crystal systems which are amenable to study by the techniques in (ii) and which will address the problems in (i). This is a complex matrix. The objectives below each contain several of the elements of this matrix but in general the philosophy is as follows.

There are four problems to be addressed: (a) the growth mechanisms for different system types; (b) the units of attachment; (c) defect and intergrowth incorporation; (d) crystal habit. The technique limitation is mainly as follows: HREM is best for silicates, aluminosilicates and titanosilicates; NMR is best for aluminophosphates but will be stretched to silicates using modern processing techniques, it is not good for paramagnetic materials; modelling is best for high-symmetry crystal systems and in particular silicates; the AFM, SEM and mass spectrometry should be amenable to all systems. It is with this in mind that the systems for study within the workpackages have been carefully chosen.



A schematic of the overall management structure is shown above left, indicating reporting and knowledge transfer pathways. Prof. Michael Anderson will assume overall coordination with specific target areas managed by a team of academic experts. PDRAs (■) will assist in the guidance of PhDs (●). The PhDs that will travel overseas (● one year in Versailles doing NMR work with Prof. Taulelle and ● one year in Sweden doing microscopy with Prof. Terasaki and Dr. Alfredsson) will have academic supervisors both at UMIST and in the host institutions. In each case the UMIST supervisor will visit the student in the host institution once during their stay. Every six months the team will produce a report and a meeting will be held at UMIST to review the project, discuss progress, monitor targets and to fine tune the work programme. This will facilitate and ensure a free flow of information between all experimentalists and theoreticians (above right).

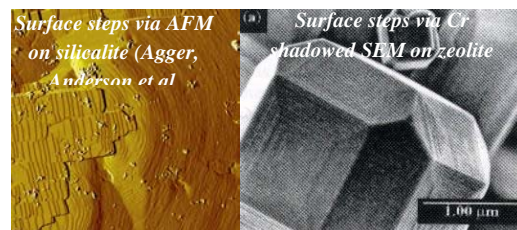
A description of the scope of each project objective with specific tasks follows.

OBJECTIVE 1: Establish breadth of possible growth mechanisms for open framework materials.

To date there has been quite detailed work on crystal growth mechanisms on the following framework systems: zeolite Y,^[1,44] zeolite A,^[2,42-44] silicalite,^[10] zeolite L,^[44] SSZ-42,^[5] ZnPO-X,^[9] MnAPO-50.^[12] This list covers both a range of framework types and also chemical makeup and includes crystals grown both with and without organic structure directing agents. However, phase space coverage is limited and it is very important to considerably expand this such that subsequent more detailed studies are able to focus on key growth phenomena rather than targeting interesting curiosities. This requires more rapid screening than hitherto achieved for a range of carefully selected crystallites. Many of these crystals we already have but many more will be synthesised.

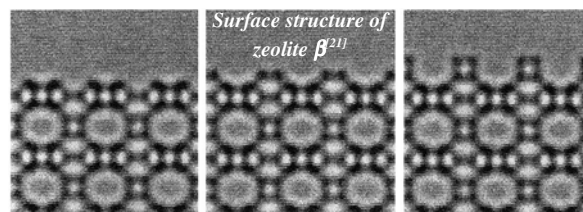
To rapidly screen crystallite surface phenomena two techniques will be used: first, high-resolution SEM on Cr-sputtered samples whereby the Cr preferentially decorates and therefore shadows surface features; second, ultra-high resolution SEM on non-coated samples – currently being developed at Hitachi and demonstrated recently by Terasaki *et al*^[46]. This will shortly be available to this project in Stockholm and should permit rapid observation of nanometer high surface features. This will be followed by extensive *ex-situ* AFM monitoring of the more interesting features observed in the initial screening. Three specific systems will initially be targeted: first, fluoride versus hydroxide synthesis of silicalite as solution speciation is known to be very different; second, synthesis of faujasite structure under conventional and reverse micelle growth conditions which substantially affects the nature of the growth units and consequent structural features; third, silicalite crystallised under continuous feed conditions with constant and known levels of supersaturation. Dr Colin Cundy at UMIST has specific expertise in this latter area which will permit understanding the role of supersaturation in the rate of specific growth processes.

- WP1A** [●●●] Synthesis of micro-porous crystals: silicates, aluminosilicates (zeolites), aluminophosphates, metal-substituted aluminophosphates, octahedral and octahedral/tetrahedral molecular sieves.
- WP1B** [●/●] Cr sample coating and FEG-SEM investigation for rapid, global determination of habit and surface topographies.
- WP1C** [●/●/●] In air, *ex-situ*, AFM imaging of samples of interest (as above) to better characterise growth features, including height measurements and checking for supplementary features not observable by FEG-SEM.
- WP1D** [●/●/●] Comparative study of fluoride and hydroxide syntheses, *e.g.* silicalite.
- WP1E** [●/●/●] Comparative study of hydrothermal and reverse micelle syntheses, *e.g.* ZnPO-X.
- WP1F** [●/●/●] Comparative study of continuous feed and batch process syntheses to determine the effects of supersaturation considerations on crystal growth. Wealth of characterised continuous feed samples to be provided by Dr Colin Cundy.



OBJECTIVE 2: Establish relationships between structure and growth mechanism.

In order to establish the precise structural make-up at the surface of a crystallite – where growth takes place – there is only one experimental technique available at present, high-resolution transmission electron microscopy. AFM yields information concerning terrace topography which, in conjunction with molecular modelling, leads to the proposal of potential layer structures but AFM cannot determine precisely at which plane a surface terminates. HREM has already been used successfully in this regard for zeolites Y^[47], L^[48] and beta^[17] and for the titanosilicate ETS-10.^[49] Surface structure can be calculated *via ab initio* methods and this forms part of objective 6, however, it is crucial to have experimental evidence in this regard. HREM will also be used to determine specific defect structures which provide invaluable clues in the elucidation of crystal growth mechanisms (this has been used very successfully in studies of ETS-10 and silicalite). Defect concentration will also be quantified using spectroscopic methods such as FTIR and NMR where a suitable signature is present.



- WP2A** [●/●] HREM studies of surface structure.
- WP2B** [●●●●] Surface layer / crystal structure relationship determination using molecular graphics, Cerius².
- WP2C** [●] NMR and FTIR of defect concentration profiles.

OBJECTIVE 3: In-situ AFM imaging.

Developing techniques for *in-situ* AFM imaging is important in order to simulate real synthesis conditions as closely as possible. This is quite a challenge because of the typical conditions (temperature/pressure/alkalinity) of synthesis of framework materials and the micro-crystalline nature of many of the resulting crystallites. Consequently, the technique will not be as widely applicable as *ex-situ* measurement. However, there are a number of important clear gel syntheses which can be carried out near ambient temperature. For instance zeolite A, zeolite Y and a number of framework phosphate syntheses. *In-situ* results will give direct access to growth kinetics and help verify the modelling methods used more widely on the results from *ex-situ* measurement. Atomistic simulation will be used to support the experimental effort. AFM aids the simulation by identifying target structures - the simulations may yield plausible atomic level structures and their energies.

- WP3A** [■] Imaging crystals under liquids.
- WP3B** [■] Studying *in-situ* crystal dissolution.
- WP3C** [■] Development of low temperature, clear gel syntheses.
- WP3D** [■] Studying *in-situ* crystal growth.

WP3E [●●●] Atomistic simulation of structure and stability of surface features.

OBJECTIVE 4: Determine the influence of templates and inhibitors / habit modifiers on growth mechanism.

Many framework materials are synthesised in the presence of organic structure directing agents that bind to the growing surface and then become clathrated inside the final crystal structure. Owing to the porous nature of these structures the crystal surfaces are highly corrugated which permits tight binding of both “templates” and habit modifiers such as polymers and carboxylic acids etc. A detailed study of the effects of such growth modifiers on detailed crystal surface topology and atomistic calculation of the energies involved should permit the determination of their influence on specific growth processes.

WP4A [✓] Investigation of surface topographical changes by FEG-SEM and in air, ex-situ, TappingMode AFM.

WP4B [✓] Establish conditions for template surface decoration in terms of concentrations and competition of different templates by atomic-resolution AFM of crystal facet decoration and calculation of equilibrium constants (conductivity measurements and particle sizing) at varying temperatures leading to binding energies.

WP4C [●●●] Calculate binding energies of templates/additives at surfaces.

WP4D [✓] Understand *c* axis control in the following uni-dimensional pore system structures: zeolite L, mordenite, AlPO-5, CoAPO-5, CrAPO-5 by atomic-resolution AFM of crystal facet decoration by inhibitors / habit modifiers, such as carboxylic acids, etc.

OBJECTIVE 5: Identify the units of attachment.

In-situ NMR^[50] in conjunction with mass spectrometry will be used to monitor solution-based chemical processes during nucleation and growth to attempt to bridge the gap between the gel and the growing crystal surface. *In situ* EDXRD measurements will be used to define the crystallisation co-ordinate for these speciation studies. Particular attention will be paid to silicate, aluminosilicate and metallophosphate materials as they contain NMR active nuclei such as ¹⁷O, ²⁷Al, ²⁹Si and ³¹P. Silicate solutions still require further NMR studies as complete assignment of ²⁹Si NMR spectra is not currently available. 2D INADEQUATE ²⁹Si NMR will be of great help to determine connectivity between different silicon sites. An NMR data processing tool recently developed in Versailles named ANAFOR^[51] will help to overcome low sensitivity of NMR response limitations and improve quality of spectra in terms of signal-to-noise ratio. ANAFOR is a computer program based on linear least squares fitting of the time-domain signal that allows significant decrease of experimental data collection time in multidimensional NMR experiments. 2D ²⁹Si experiments should become routine.

Mass spectrometry is a complementary technique to NMR for speciation^[45]. It has the advantage of being very fast and consequently the timescale for the experiment can potentially be much faster than NMR. This is especially true for silicon which is notoriously difficult in NMR owing to low natural abundance of the ²⁹Si isotope. Chemical signatures need to be deconstructed from fragmentation patterns which makes interpretation slightly more challenging than NMR.

For both the NMR and MS experiments it will be important to differentiate between spectator species and the species of attachment. This can often be achieved through dissolution experiments rather than crystal growth experiments which, owing to relative reaction rates, results in high solution concentrations of the units of attachment.

WP5A [●] *In-situ* NMR of dissolution and growth of silicates, aluminosilicates and aluminophosphates.

WP5B [●] *In-situ* Mass spectrometry of dissolution and growth of silicates, aluminosilicates and aluminophosphates.

OBJECTIVE 6: Calculate attachment energies and crystal surface energies.

Atomistic simulation methods have proved to be an invaluable tool in the quest to understand the complex process of crystal growth in microporous materials. Notable successes in this field include the prediction of surface structure^[52] and of stable growth units in solution^[17], and also the successful synthesis of targeted materials using computer designed templates^[34]. There is now an opportunity to connect these three distinct components of the growth process in order to understand the phenomenon of growth. Through this network of researchers, our work will directly feed into the AFM, HREM and NMR lead programs. In addition, the simulation work will complement and provide accurate parameterisation for the mesoscopic growth software planned by Agger in objective 7. Key elements of our research program will focus upon 1) determining the reaction energy and rate of attachment for growth units at terrace, step and kink sites 2) modelling of line and point defects (including stacking energies) within nanoporous materials 3) exploring how the polarity and ionic strength of the solvent changes the stability of growth units in solution and the reaction pathway with the crystal surface 4) the role of extra-framework cations in condensation reactions between the crystal and growth unit.

In 1), classical constrained free energy minimisation calculations will be undertaken to assess the binding energies of reactive species upon the terrace, step and kink sites. In deliverable 2) we will provide complementary research to objective 8. Specifically, we will use computer simulation methods to investigate complex defects in nanoporous materials, focusing on ETS-10 and zeolite Beta. Recent work on nanosized defects in zeolite L^[18] using atomistic methods attests to the applicability of this technique to provide quantitative and mechanistic insight into how nano-sized defects are incorporated into the lattice. Using a combination of classical and quantum mechanical methods, it will be possible to determine, the ease with which defects can be included and this can be utilised to provide estimates of the defect concentrations under variable temperature and pressure regimes. This proven computational approach will allow us to investigate the origin of, for example, stacking

faults within materials. Using this information, we will be able to direct synthesis programmes to particular regions in the phase map that will result in low defect materials.

Allied to objective 4, we will undertake a series of studies on prediction of morphology, concentrating on understanding and predicting how inhibitors can be utilised to manipulate crystal shape for a desired purpose. Each student will focus upon different topical materials that will include ALPO-5, Mordenite and zeolite L. For example, in zeolite L, access to the 12MR, which is exposed on the (001) surface, should be maximised for catalytic applications. To engineer a platy crystal habit with (001) as the most morphologically important face, the growth of the (001) face must be slowed. By modifying ZEBEDDE we will be able to identify inhibitors with particularly strong binding to the (001) face, temporarily blocking the key points of attachment upon the surface. These inhibitors will drastically slow the growth of the (001) face, ensuring that plate-like crystals are formed. Solvation effects will be explored using explicit solvent bath schemes to measure how the stability of surfaces is affected by the presence of polar media.

Understanding the formation of small-units in solution and how they react with crystal surfaces encapsulates the theme of item 4) and builds upon the findings of 1) (WP6A). Here, classical based work will be extended by full quantum mechanical investigation to address the enthalpy of reaction of small units in solution and with zeolite crystal surfaces using plane-wave and local-orbital based DFT methods. The findings will be crucial to our understanding of mechanism pathway and mark an important development in the goal to rationalise the nucleation to crystallisation transition.

Each of the three PhD students will be supervised individually by each of the co-investigators, working on seven distinct materials; ETS-10, mordenite, ALPO-5, zeolite Beta, zeolite Y, zeolite L and zeolite A. To exploit the individual expertise of the co-investigators, each PhD student will spend a period of their research within each investigators laboratory. Specifically, SCP will coordinate free-energy work, DWL will supervise cation templating and BS will coordinate the surface structure determination and morphology prediction elements of the student's research programmes. This work will be tightly coordinated with the NMR, AFM and HREM studies to ensure synchronous and synergistic research. We will use a combination of classical and electronic structure methods to perform our simulation studies, using METADISE^[53], MARVINS^[54], DL_POLY^[55] and CASTEP^[56]. This concert of techniques will give us a holistic understanding of the growth process, from solution species to the assembly of nanoscale sized crystal faces.

WP6A [●●●] Calculating the free energy and rate of attachment of growth units to flat and stepped surfaces.

WP6B [●●●] Understanding the origin of line and point defects within nanocrystalline solids.

WP6C [●●●] Study the effect of solvent and inhibitors on the growth process and crystal morphology.

WP6D [●●●] Determine contribution of cations to crystal growth mechanism.

OBJECTIVE 7: Bridge the gap between experiment and theory via simulation of AFM and SEM images.

The ability of AFM, and more recently SEM, to provide hitherto inaccessible information on the surface structure of synthetic microporous materials has led to the proposal of some crystal growth mechanisms of open framework materials. Whilst similarities abound between the features observed on different structures, profound differences also exist – computer simulation techniques based on original work by Stranski^[57] have thus been employed to understand the complexity observed. 2D simulations of growth layers have provided insight into the inherent link between nutrient surface attachment energies, which are modelled as attachment probabilities, and the layer topographies observed.^[4] In this project we will create 3D models capable of predicting not only surface topography but also overall crystal morphologies with parameterised input based on atomistic calculations.^[58] This will allow extraction of individual growth probabilities and ultimately attachment energies from the microscopy work. The culmination of this work will result in an integration of the individual simulations into a flexible package, able to simulate crystal growth, with or without defect inclusion, across the spectrum of crystal symmetries and crystal morphologies.

WP7A [●] Creation of individual simulations to model habit and surface topography from experimental data.

WP7B [●●●] Incorporation of intergrowths and defects in model.

WP7C [●] Development of a global formalism allowing creation of a simulation package able to model mechanisms for different crystal symmetries.

WP7D [●●●●] Determine attachment energy / simulation probability relationships and sphere of influence.


WP7E [●●] Determine diffusion limitation vs thermodynamic limitation.

WP7F [●] Develop methodologies for computation and rendering of realistically sized crystals

OBJECTIVE 8: Exert control over a crystal growth process.

Ultimately, the knowledge base generated by objectives 1-7 will enable us to exert control over the crystallization of specific microporous materials. An example is the titanosilicate material ETS-10, whose structure can be considered as a series of layers comprising of interleaved silicate-clad titanate chains and 12-ring pores. The alternating nature of the chains and pores offers the possibility of two distinct surface nucleation sites. Subsequent growth at these two sites results in either the layers growing in registry with each other, or the contrary, which leads to the formation of line defects (stacking faults). One of the most interesting potential applications of ETS-10 is as an opto-electronic material owing to the quantum wire-like nature of

the titanate chains. However, successful exploitation of these properties relies on elimination of, or reducing to very low levels, these line defects. We propose that using the knowledge gained here (objectives 1-7) we will be able to devise a suitable synthesis strategy that will allow the surface nucleation to be controlled so as to reduce the occurrence of faulting. Similar structural defects occur in a number of other materials – for example mordenite and ferrierite – that may also be amenable – depending on project progress – to such a treatment.

WP8A [] Control of line defects in ETS-10 – or other system chosen in final year of project.

RELEVANCE TO BENEFICIARIES

Application-driven technological demands require vastly superior nano-scale control of structure relative to current state-of-the-art. The phenomena of nucleation and crystal growth are inherent to exerting such control. Consequently targeting an improved understanding of these phenomena is vital. The benefits (and predicted impact areas) will include: overcoming crystal size limitations and improving crystal purity (opto-electronics, membrane technology, separations, defense); controlling intergrowth structures and crystal habit (catalysis and water treatment); more cost-effective routes to existing but prohibitively expensive known structures (sensors, batteries, catalysis and biocatalysis).

DISSEMINATION AND EXPLOITATION

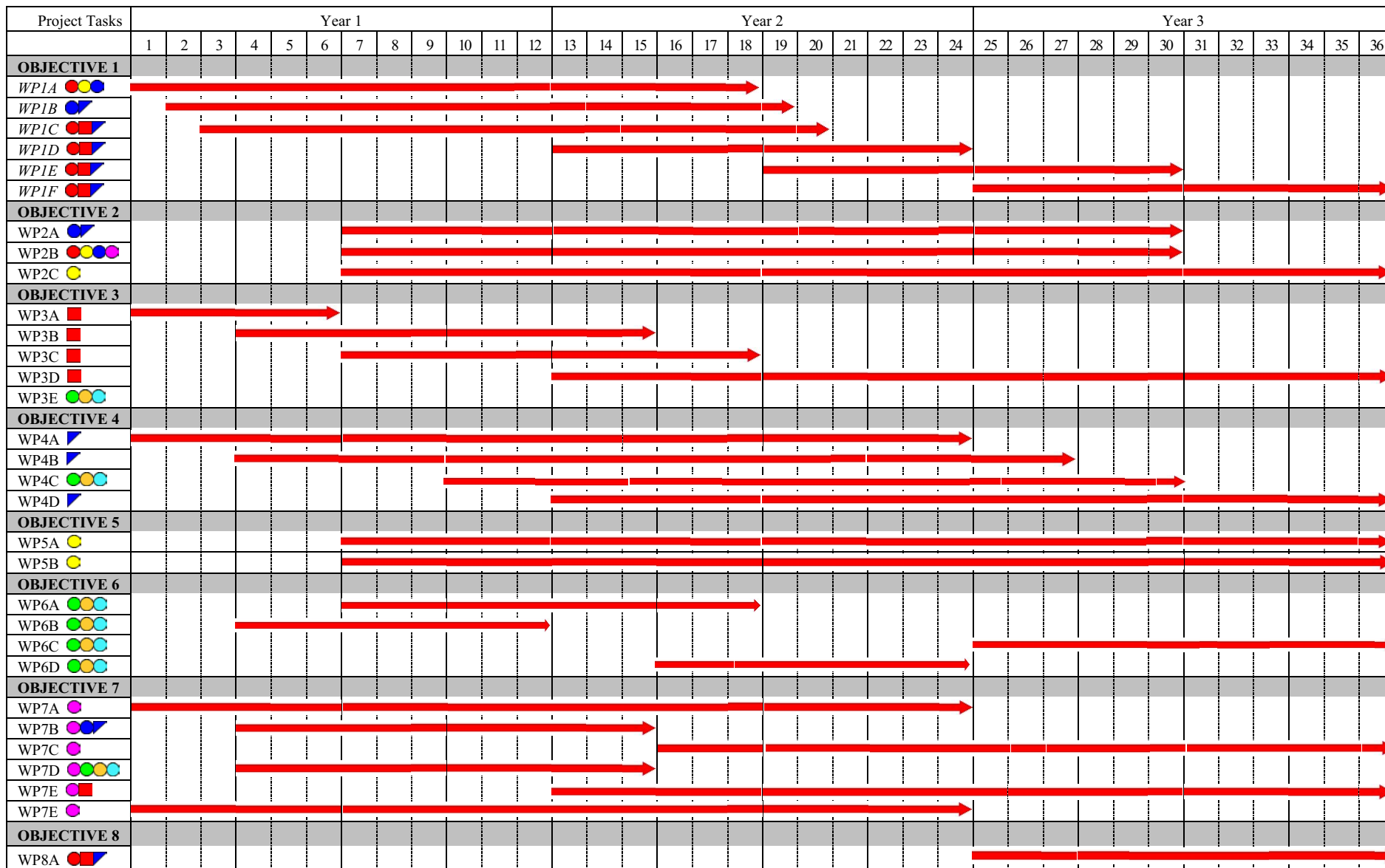
The main route for dissemination of scientific property will be through the open literature, *via* presentation at both national and international conferences, specifically the BZA, FEZA and IZA and via a dedicated web site. The novel nature of this work should be ideal for publication in high impact factor international journals such as *Nature*, *Science*, *Angew. Chem.*, *J. Amer. Chem. Soc.*, *Phys. Chem. Chem. Phys.*, *J. Phys. Chem.*, *J. Cryst. Growth*, *J. Mater. Chem.*, *Chem. Mater.* and *Ultramicroscopy*. UMIST, through UMIST Ventures Ltd., is very keen to patent inventions and any major new experimental designs emanating from this work would be considered for patenting.

JUSTIFICATION OF RESOURCES

The total amount of funding requested is £968,000 which will support the research of over 19 researchers and academics in a truly unified project. We believe that by bringing together leading researchers in the field of microporous materials to tackle a major scientific problem, our proposed network represents outstanding value for money (less than £50k per researcher) and is likely to make far more impact than individual researchers working in isolation.

The main cost on the project is the personnel cost for a large team with interrelated expertise. This will involve 7 PhDs, 1.5 PDRA and technical support. Staff numbers and seniority have been carefully chosen to ensure the team is able to carry out the wide range of activities to the necessary level of competence and within the timeframe of the project. In this respect one PDRA and PhD student will work on AFM and synthesis with the PDRA concentrating more on *in situ* AFM development and the student on *ex situ* measurements. One PhD student will work on solution phase speciation using NMR and mass spectrometry – this student will also perform *in situ* XRD measurements at station 16.4, Daresbury (for which time will be requested separately) to define the crystallisation co-ordinate for their speciation studies. One PhD student and 0.5 PDRA will concentrate on electron microscopy measurements of surface structure. This is a complex technique requiring the full dedication of separate personnel. One PhD student will carry out computer simulation of crystal morphology and topography in order to extract kinetic and thermodynamic information from the experimental data. Finally, three PhD students will work on classical and *ab initio* modelling of surface structure, binding energies and rates of attachment of growth units and cation templating studies. The experimental synthetic work will be supported by 20% of an experienced technician. This is the minimum number of personnel to perform this complex range of tasks.

This proposal relies on importing some knowledge from overseas in terms of a) high-resolution TEM and ultra-high resolution SEM from the groups of O. Terasaki and V. Alfredsson and b) *in situ* NMR of crystallisation from F. Taulelle. The idea is to establish a knowledge base that can be retained in this country within the UCMM after the end of this project. This necessitates two of the PhD students carrying out 1/3 of their studies abroad for which travelling and a modest extra subsistence is requested. Travelling is also requested to hold 6 monthly project meetings of all members in Manchester. Attendance at one international conference is requested for the team as well as annual participation by the students at the British Zeolite Association Conference. Equipment for the project comprises: an AFM with high-resolution optical microscope, for locating micron-sized crystals and variable temperature capability for *in situ* studies; AFM probes; a Cr sputterer for the high-resolution SEM studies at UMIST; We have requested additional monies to provide 1 Linx-based high-performance workstation for each simulation PhD student. These machines will be dedicated computer resources for undertaking the numerically intensive simulation work. Running and access costs are also requested for NMR, MS and TEM/SEM at UMIST.



Work Package duration

ANNEXE 1: CVs of named staff and visiting researchers

**CURRICULUM VITAE
RICHARD JOHN PLAISTED**

ADDRESS: 10, Rockfield Drive,
Helsby,
Warrington.
WA6 9AR

TELEPHONE 01928 723694

DATE OF BIRTH 16th May 1942

NATIONALITY British

MARITAL STATUS Married with two children

PROFILE**Research**

I have been actively engaged in research in chemistry and materials science since 1960. A feature of all my work has been collaboration in joint projects across a range of activities and working in a flexible manner on a range of different projects simultaneously. I am accustomed to working to BS5750 quality standards and within COSHH and SHE regulations.

Teaching and lectures

I have presented work on synthesis of zeolites, evaluation of zeolite synthesis and silicate solution chemistry at symposia both within ICI and at UMIST. I have also lectured on the postgraduate course on Microporous Materials.

EDUCATION

1960 Saltley Grammar School, Birmingham
'A' level in Physics, Chemistry and Mathematics
'S' level in Chemistry and Mathematics

1962 Gwent College of Further Education, Newport, Gwent
HNC Chemistry
A levels in Pure Mathematics and Applied Mathematics

1965 University of Manchester, Faculty of Technology
B.Sc (Hons) Chemistry

CAREER SUMMARY

1960-1962 British Nylon Spinners Ltd.
Pontypool, Gwent.
Laboratory Assistant: Work on synthesis of polyamide intermediates. Processing of polyamides by melt and solution spinning.

1965-1966 Dunlop Chemical Products Ltd
Birmingham
Research Chemist: Evaluation of emulsion polymerisation methods with acrylic systems.

1966-1994 ICI Chemicals and Polymers Ltd
Research and Technology Dept.
Runcorn, Cheshire.

1966-1975 Experimental Officer: Work on carbon fibres and films. Synthesis, processing and post treatment of acrylic fibres to improve performance. Investigations of phosphate glass systems.

1975-1987 Senior Experimental Officer: Development of methods for investigation of silicate and alumino-silicate solution chemistry. Developed inorganic phosphate polymers to semi-tech scale. Synthetic work on phosphorus-nitrogen and sulphur-nitrogen systems.

1987-1994 Research Scientist
Planned and implemented project work to develop new and improved inorganic microporous materials by increased understanding of the synthetic mechanisms. Identified and introduced new experimental and evaluation techniques, equipment and methodology. Maintained a safe working environment to comply with COSHH regulations.

1994 – present UMIST

Research Associate: Work in fields of microporous and mesoporous materials. Evaluation of crystallisation of inorganic systems. Responsibility for running Microporous Materials laboratory.

Awarded M Phil in 2003

INTERESTS AND OTHER INFORMATION

I play chess and bridge on a regular basis. I have been league conductor for my local chess league for the last twenty years and have represented my county on a fairly regular basis. I am interested in music, reading and enjoy walking. I hold a full driving licence. I have some knowledge of scientific German and French.

PAPERS PUBLISHED

N.H.Ray, R.J.Plaisted, W.D.Robinson

Oxide glass of very low softening point: Part IV Preparation and properties of ultraphosphates containing boric oxide
Glass Tech. **1976**, 17, 66.

N.H.Ray, R.J.Plaisted

Trimethylation of Zeolites: Evidence for presence of adjacent aluminium atoms
J. Chem. Soc. Dalton Trans., **1981**, 1260.

N.H.Ray, R.J.Plaisted

The constitution of aqueous silicate solutions
J. Chem. Soc. Dalton Trans., **1983**, 475.

C.S.Cundy, L.Griffiths, R.J.Plaisted

Equilibrium studies of silicate anions in aqueous solution by dynamic ²⁹Si NMR spectroscopy
J. Chem. Soc. Dalton Trans., **1986**, 2265.

C.S.Cundy, M.S.Henty, R.J.Plaisted

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Zeolites, **1995**, 15, 342-352.

C.S.Cundy, M.S.Henty, R.J.Plaisted

Zeolite synthesis using a semi-continuous reactor. Part I: Controlled nucleation and growth of ZSM-5 crystals having well defined morphology.
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C.S.Cundy, M.S.Henty, R.J.Plaisted

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S.M.Holmes, V.L.Zholobenko, A.Thursfield, R.J.Plaisted, C.S.Cundy, J.Dwyer

In-situ FTIR study of the formation of MCM-41
J. Chem. Soc. Faraday Trans., **1998**, 94, 2025-2032.

C.S.Cundy, R.J.Plaisted, Z.P.Zhao

Remarkable synergy between microwave heating and the addition of seed crystals in zeolite synthesis- a suggestion verified.
Chem. Commun., **1998**, 1465-1466.

Z.P.Zhao, C.S.Cundy, R.J.Plaisted, J.Dwyer

Potential of microwave heating in [Al]ZSM-5 synthesis
Proc. 12th Internat. Zeolite Conf., Mater. Res. Soc., **1999**, 1591-1594.

S.M.Holmes, C.Markert, R.J.Plaisted, J.O.Forrest, J.R.Agger, M.W.Anderson, C.S.Cundy, J.Dwyer

A novel method for the growth of silicalite membranes on stainless steel supports
Chem. Mater., **1999**, 11, 3329-3332.

S.M.Holmes, M.Schmitt, C.Markert, R.J.Plaisted, J.O.Forrest, P.N.Sharratt, A.A.Garforth, C.S.Cundy, J.Dwyer

Zeolite-A Membranes for Use in Alcohol/Water Separations
Chem. Eng. Res. Des., **2000**, 78, 1084-1088.

C.S.Cundy, J.O.Forrest, R.J.Plaisted,

Nucleation processes in zeolite synthesis revealed through the use of different temperature-time profiles
Stud. Surf. Sci. and Catal., **2001**, 135, p. 140.

CURRICULUM VITAE**Osamu Treasaki**

ADDRESS Arrhenius Laboratory,
Stockholm University
Stockholm, S-106 91,
SWEDEN

TELEPHONE +46 (0)8 162379

DATE OF BIRTH 16th February 1943

NATIONALITY Japanese

MARITAL STATUS: Married since 1968 with one daughter and two sons.

EDUCATION:

Department of Physics, Faculty of Science, Tohoku University, B. Sc. with Honors, 1965.
Graduate course, Department of Physics, Tohoku University, MSc. 1967.

TITLES: Doctor of Science, Tohoku University, 1982.

OCCUPATION:

1967 – 1994 Research Physicist, Department of Physics, Faculty of Science, Tohoku University.
1994 – 2002 Associate Professor, Head of the Microstructure Physics Group, Department of Physics, Graduate School of Science, Tohoku University.
1995 – 2002 Associate Prof. Centre for Interdisciplinary Research, Tohoku Univ.
1996 – 2001 Research Director, Core Research for Evolutional Science & Technology (CREST), Japan Science and Technology Corporation (JST).
2002 – 2003 Professor, Dept. Phys., Grad. School of Science, Tohoku Univ.

PRESENT POSITION: Professor of Structural Chemistry, Arrhenius Laboratory, Stockholm University.

GUEST RESEARCH FELLOWSHIPS

Oct 1982 – Mar 1984 Guest Research Fellow of the Royal Society (UK).
Department of Physical Chemistry, University of Cambridge.
Sep 1988 – Dec 1988 Guest Prof. of NFR, Inorganic Chemistry II, Univ. of Lund.
1996 – Present Guest Professor, Jilin University, China.

SCIENTIFIC AWARDS

1964 Y.S. Kuno Prize, Honor Prize of Tohoku University.
1982 First Place, International Metallographic Exhibit in the electron microscopy-transmission class (International Metallographic Society and American Society for Metals).
1993 Seto Award, Award of Japanese Society of Electron Microscopy.
1996 Daiwa Adrian Prize, Daiwa Anglo-Japanese Foundation, London.
2001 The Best Paper Award, Japanese Society of Electron Microscopy.

INTERNATIONAL COMMISSIONS

Editorial Board Member of Microporous and Mesoporous Materials, 2001-
Council Member of International Zeolite Association (IZA), 2001-
Structure Committee Member of IZA, 2001.

PUBLICATIONS

218 peer reviewed publications and 2 books.

CURRICULUM VITAE

Name: Viveka Ingegerd Alfredsson

Date of birth: 6 April 1963

Address: Physical Chemistry 1, Lund University, P. O. Box 124, 221 00 Lund, Sweden

Telephone: +46 46-222 81 55

Email: viveka.alfredsson@fkem1.lu.se

Home address: Skördevägen 2E, 227 38 Lund, Sweden

Present position: Assistant Professor at Physical Chemistry 1, Lund University, since February 1998

Former positions: Research Engineer at Sandvik Coromant, Stockholm, Sweden from August 1996-January 1998

Postdoc at Inorganic Chemistry Lund University, Sweden from February 1996-July 1996

Postdoc at Department of Chemistry, UMIST, UK, from February 1995-January 1996

Education: Master of Science in Engineering, 11 October 1988, Lund University, Lund, Sweden.

Doctor of Philosophy in Engineering in Inorganic Chemistry, 28 October 1994, Lund University, Lund, Sweden.

Publications (1994-2003)

1. High-resolution transmission electron microscopy of mesoporous MCM-41 type materials

Alfredsson, Viveka; Keung, Michael; Monnier, Alain; Stucky, Galen D.; Unger, Klaus K.; Schueth, Ferdi
J. Chem. Soc., Chem. Commun. (1994), (8), 921-2

2. Zeolites – a High Resolution Electron Microscopy Study.

Alfredsson, V. Thesis, Lund, (1994)

3. Fine structures of zeolites: Defects, interfaces and surface structures. An HREM study

Terasaki, O.; Ohsuna, T.; Alfredsson, V.; Bovin, J-O.; Carr, S. W.; Anderson, M. W.; Watanabe, D.
Stud. Surf. Sci. Catal. (1994), 83(ZEOLITES AND MICROPOROUS CRYSTALS), 77-84

4. The platinum agglomeration in the {111}-twin planes of the zeolite FAU

Alfredsson, Viveka; Terasaki, Osamu; Blum, Zoltan; Bovin, Jan-Olov; Karlsson, Gunnel
Zeolites (1995), 15(2), 111-16

5. Structure of MCM-48 Revealed by Transmission Electron Microscopy

Alfredsson, Viveka; Anderson, Michael W.
Chem. Mater. (1996), 8(5), 1141-6

6. Observations on the role of crown ether templates in the formation of hexagonal and cubic polymorphs of zeolite Y

Ohsuna, Tetsu; Terasaki, Osamu; Alfredsson, Viveka; Bovin, Jan-Olov;

Watanabe, Denjiro; Carr, Stuart W.; Anderson, Michael W.

Proc. R. Soc. London, Ser. A (1996), 452(1946), 715-40

7. TEM-tomography of FAU-zeolite crystals containing Pt-clusters

Bovin, Jan-Olov; Alfredsson, Viveka; Karlsson, Gunnel; Carlsson, Anna; Blum, Zoltan; Terasaki, Osamu

Ultramicroscopy (1996), 62(4), 277-281

8. The First Large-Pore Vanadosilicate Framework Containing Hexacoordinated Vanadium
João Rocha, Paula Brandão, Zhi Lin, Michael W. Anderson, Viveka ALFREDSSON, Osamu Terasaki
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9. Cubosome Description of the Inorganic Mesoporous Structure MCM-48
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10. Deposition of hard crystalline Al₂O₃ coatings by bipolar pulsed d.c. PACVD
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11. The Effect of Stirring on the Synthesis of Intergrowths of Zeolite Y Polymorphs
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12. Triblock copolymers as templates in mesoporous silica formation; structural dependence of polymer chain length and synthesis temperature
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13. Macroscopic alignment of silver nanoparticles in reverse hexagonal liquid crystalline templates.
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Nanoletters, 2002, 2, 1403-1407

14. Influence of the block length of triblock copolymers on the formation of mesoporous silica.
Flodström, Alfredsson
Microporous and Mesoporous Materials, 2003, 59, 167-176

15. Formation of a new Ia3d cubic meso-structured silica via triblock copolymer assisted synthesis.
Flodström, Alfredsson, Källrot
J. Am. Chem. Soc. 2003, 125, 4402-4003

CURRICULUM VITAE

Francis Taulelle

Personal situation

1951 Born January 12, Sousse (Tunisia) French citizenship.

Married June 3, 1972 in Paris with Dominique Péré- two children: Djamilia born in 1974 and Michaël born in 1976.

Studies

1969 Baccalauréat

1969-1972 Mathématiques supérieures and mathématiques spéciales, Marcellin Berthelot Saint Maur

1972-1977 Student at Ecole Normale Supérieure de Cachan

1972-1974 Graduated in Physical Chemistry, Orsay University

1975 Master (DEA) in Physical Chemistry. University Pierre and Marie Curie, Paris

1976 Master (DEA) in Analytical Chemistry University Pierre and Marie Curie, Paris and Institut National Sciences et Techniques Nucleaires, Saclay

1983 PhD (Docteur d'Etat) in Analytical Chemistry

Title: Etude de la basicité de l'ion oxyde dans NaCl-AlCl₃ fondu à 175°C et étude de l'influence du cation Mⁿ⁺ sur les propriétés spectroscopiques et thermodynamiques des mélanges MCl_n-AlCl₃ fondus (M = Li, Na, K, Sn, N-Butylpyridinium).

Career

1972-1977 Student at Ecole Normale Supérieure de Cachan

1977-1978 CEA Fellowship in radio-chemistry, Institut National Sciences et Techniques Nucleaires, Saclay

CNRS

1978 **Research Associate (second class) at CNRS Chemistry Department**

in Pr. Tremillon's Laboratory : Laboratoire d'Electrochimie Analytique et Appliquée, Ecole Nationale Supérieure de Chimie de Paris. Main research topic : Molten salts, electrochemistry and Raman Spectroscopy.

1981-1982 On leave for one year at Michigan State University, East Lansing Michigan in Pr. Popov's group

1983 **Research Associate (first class) at CNRS Physical Sciences for Engineering Departement**

in Pr. Papon's Laboratory : Laboratoire des Dispositifs Infra-rouge et Physique Thermique Ecole Supérieure de Physique et Chimie Industrielle, Paris. Main research topic : Solid state NMR and instrumentation.

1986 **Research Associate (first class) at CNRS Chemistry Department**

in Pr. Livage's Laboratory : Laboratoire de Chimie de la Matière Condensée University Pierre and Marie Curie, Paris. Main research topic : Multinuclear NMR of Liquids and Solids of Inorganic Chemistry in Paris and co-development of the NMR group in High temperature NMR in Orleans (6 years from 1986 to 1992).

1990 On leave for one year at **Bruker Karlsruhe**, Application Laboratory. Main Activity : Instrumentation development of high temperature NMR.

1992 **Research Directeur (second class) at CNRS Chemistry Department**

and move to the mixed laboratory « Université Louis Pasteur-Bruker-CNRS » in Strasbourg

1994 **Director of NMR and Solid State Chemistry laboratory** University Louis Pasteur in Strasbourg.

2001 Start a new group In Versailles Saint Quentin University in Institut Lavoisier Directed by Pr. Ferey, while keeping the group in Strasbourg.

2002 **Research Directeur (first class) at CNRS Chemistry Department**

Supervising and contract management

I have directed C. Gerardin CNRS Research Associate, C. Huguenard, Lecturer at University Louis Pasteur, and M. Haouas CNRS Research Associate.

I supervised 5 PDRAs.

I supervised 13 PhDs, 3 shared between two Universities.

I have housed 10 doctorats for NMR part of their PhD from different French laboratories.

I supervised students: 4 Masters (DEA), 10 maitrise and 3 licence in mathematics, physics and chemistry, 2 in Technical University Institute (IUT in physical measurement).

I supervise an NMR specialist taking care of the NMR spectrometers and data processing development.

I had been managing 9 academic grants, 2 European Contracts and 7 Industrial contracts (Rhône-Poulenc, Michelin, IFP, Total) and participated in 2 cooperative research groups (GDR) (GDR Microporous oxyfluorinated syntheses and GDR Chalcogenures).

I was elected responsible for finances of the Chemistry Department at Louis Pasteur University from 1997 to 1999.

Scientific activities

I have published 117 papers and 2 Patents (1 International and 1 European).

I have presented work on 76 occasions: 23 international conferences, 21 national meetings or summer schools, and 33 seminars in both French and foreign universities or to Industry.

My main research topics are:

Crystallography of Inorganic nanoporous materials and in-situ NMR
NMR Crystallography, methodology and NMR instrumentation.

Awards

French Science Academy Prize «Paul Pascal» 1999

ANNEXE 2: Quotations

QUOTATION

Veeco Instruments Ltd, Nanotech House, Anderson Road, Buckingway Business Park SWAVESEY, CAMBRIDGE CB4 5UQ
 Phone: 01954 233900
 Fax: 01954 231300

To: **UMIST**
 Department of Chemistry

Quotation No. 0212242S
 Date: 19th December 2002

Phone: 0161 928 6508
 Fax: 0161 200 4559
 Attn: Prof. Mike Anderson

Quotation Valid for 30 days from date of issue

Item	Qty.	P/N	Description	Price
1	1	NS4-01	<p>NanoScope IV SPM Control Station</p> <p>The NanoScope IV is the most advanced SPM controller available, providing speed, sensitivity, resolution and functionality enhancements for existing and future Veeco SPMs, while retaining all the functionality of the industry-standard NanoScope IIIa.</p> <ul style="list-style-type: none"> • Requires microscope and accessories appropriate for your application. Microscopes must be NanoScope IV-compatible to support full functionality. • Up to 10X faster topographical scanning and PhaseImaging in air with TappingMode+™ than provided by conventional SPM controllers. • Requires micro-actuated cantilevers (Model DMASP) for fast scanning. Standard cantilevers can be used for scanning at conventional rates. • Includes Quadrex™ Extender Electronics with on-board lock-in amplifier for quantitative PhaseImaging™, improved accuracy, and enhanced image contrast. • Provides OneScan™ imaging with more data points per scan line (≥4000) for the highest resolution available. Allows zooming on large scans while maintaining nano-scale lateral resolution, without the need for repetitive smaller scans. • Q-control for enhanced force control, sensitivity and image contrast, and for studying tip-sample interactions. • User-available, low-noise analog feedback loop for some custom applications. • High-speed DSP and SPM-computer interface electronics • Six analog-to-digital converters (ADCs, four user-available). • Four digital-to-analog converters (DACs) dedicated to Quadrex, and four DACs for other dedicated and user applications. • Allows easy access to line sync (end-of-line), frame sync (end-of-frame), and Quadrex lock-in oscillator reference signal. • High-speed serial interface for improved hardware/software communication. • Windows NT-based SPM imaging software, including comprehensive image analysis. 32-bit dual monitor color display video with effective total resolution ≥2048x768 pixels. • Extremely flexible for adaptation to user-designed microscopes and/or custom applications. • Extensive and expanded real-time control of feedback and other parameters. Gives the user the freedom to design and execute novel SPM experiments with the advantage of the NanoScope's precision and reliability. • Pentium tower-style PCI computer with twin monitor • Includes four micro-actuated probes (Model DMASP) 	£87,903

QUOTATION

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Item	Qty.	P/N	Description	Price
2	1	Bio2-Z2	<p>BioScope Atomic Force Microscope</p> <ul style="list-style-type: none"> • Designed specifically for life sciences and biotechnology, but useful for many other applications. • Performs all major AFM imaging techniques and modes including contact and non-contact atomic force, lateral force, TappingMode (air and fluid), and force modulation. • The standard Extender Electronics Module (Model PHASE-D01) or Quadrex Extender Electronics (Model Quadrex) is strongly recommended for the best possible images, including phase/frequency detection and surface potential measurements. • Integrates an SPM head and rigid stage with inverted optical microscope. Supports simultaneous bright field, fluorescence, and confocal imaging; phase contrast, Nomarski/DIC and other transmitted light techniques can be performed after removal of the light-weight AFM unit. The AFM unit can be removed and replaced in seconds to within a few microns of its original scan position. • Equivalent magnification range of 25X to 10⁷X. • Designed for use with Zeiss Axiovert Inverted Optical Microscope Models 100/135/200, Olympus Model IX70, or the Nikon Diaphot Models 200, 300, TE200, and TE300 (optical microscope not included). • Scanning cantilever can be viewed on axis during AFM scans via inverted microscope optics. • Full 16-bit resolution on all axes for all scan sizes and offsets. • Samples can be imaged in air or <i>in situ</i> using Fluid Cantilever Holder (included, Model BFCH, see below). • CE compliant. • Includes vacuum sample holder for holding microscope slides (25 x 75mm), cover slips (25 x 25mm) and petri dishes (60mm). Vacuum pump and vacuum accessories are also included. Silicone vibration pad provided. Integrated Acoustic/Vibration Isolation System (Model ISBIO, below) strongly recommended. • Includes 20 Silicon Nitride Probes (Model DNP-20), and 10 Tapping Mode Etched Silicon Probes (Model RTESP). • Requires stage selection from among Manual Standard Stage (Model BIOMS), Manual Precision Stage (Model BIOMP), or Motorized Precision Stage (Model BIOMO; see BioScope Options and Accessories below). • Requires NanoScope IIIa or IV SPM Control Station and Dimension SPM Microscope Head (Model DAFM). 	£16,935
3	1	DAFM	<p>Dimension SPM Microscope Head</p> <p>SPM/AFM scanner with horizontal imaging area of 90µm x 90µm nominal maximum and a vertical range of 6µm nominal maximum. Includes tip holder and TrakScan optical lever position detection system. CE compliant.</p>	£21,452

QUOTATION

Veeco Instruments Ltd, Nanotech House, Anderson Road, Buckingway Business Park SWAVESEY, CAMBRIDGE CB4 5UQ
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 Fax: 01954 231300

Item	Qty.	P/N	Description	Price
4	1	BIOMO	Motorized Precision Stage for BioScope AFM <ul style="list-style-type: none"> Motorized Precision Stage offers motorized sub-micron resolution. Joystick provides fine motion and directional control for precise positioning of sample features beneath AFM probe. Also allows positioning from outside an acoustic enclosure (e.g., with Model ISBIO-2) Available for supported Nikon, Olympus and Zeiss inverted optical microscopes. 	£11,452
5	1	ISBIO-2	Integrated Acoustic/Vibration Isolation System for BioScope AFM <ul style="list-style-type: none"> Provides acoustic isolation and increased vibration isolation. Technical Manufacturing Company Air Table; pneumatic table with caster assembly. Vibration isolation platform enclosed within acoustic hood. Additional space provided for peripheral equipment, such as video systems, micromanipulators, fluid pumps, etc. Extra cable ports provided for customized applications. Call for limitations on the height of frame spacers used with this hood. See Facilities Requirements for weight, dimensions and other important information. 	£13,710
6	5	DNP-S20	Silicon Nitride Probes Oxide-sharpened SiN probes, 4 levers per probe for Dimension (Qty. 20)	£610
7	2	RTESP7	TappingMode Etched Si Probes, rotated tip (Qty 70)	£1,764

Total System List Price

£153,826

Prices: Given in £ Sterling (GBP), and are excluding VAT.

Veeco reserves the right to adjust these prices before a Purchase Order is received should there be a USD:GBP exchange rate change of >5% from the date of issue of this quotation.

Delivery: DDP UMIST, UK, estimated at 10 weeks ARO

Payment Terms: 90% delivery, 10% installation 30 days to approved account holders subject to credit rating.

Warranty: 12 months parts and labour, On-site

Installation & Training: Carried out over a two day period, with a third day held over for advanced user training.

Signature:

Dr. Stephen J. Badger
 Sales Engineer – UK North

QUOTATION

Veeco Instruments Ltd, Nanotech House, Anderson Road, Buckingham Business Park SWAVESEY, CAMBRIDGE CB4 5UQ
 Phone: 01954 233900
 Fax: 01954 231300

Optional Items

Item	Qty.	P/N	Description	Price
6	1	BIOFHTR	<p>Fluid Heater for the BioScope AFM with Zeiss or Nikon Optical Microscope</p> <ul style="list-style-type: none"> Provides in-situ heating and temperature control up to 60°C for fluid-filled 60mm Petri dish. For contact or TappingMode operation in fluid with fluid cantilever holder (Model BFCH, supplied with BioScope) using Model DNP or DNP-S probes <u>only</u>. Nominal temperature variability is $\pm 0.5^{\circ}\text{C}$ in AFM/optical viewing area. $< 2^{\circ}\text{C}$ (1°C typical) overall temperature gradient inside viewing area as measured at 37°C. Includes heated sample holder with integrated temperature sensor (used in place of standard sample holder supplied with BioScope), external thermistor (temperature sensor) for direct monitoring of fluid temperature, evaporation covers (2), and heater controller with readouts for temperature set point, sample holder temperature, and thermistor (fluid) temperature. 	£9,677
7	1	BIOFHC	<p>Fluid Heater/Cooler and Perfusion Chamber for the BioScope AFM</p> <ul style="list-style-type: none"> Provides in-situ temperature-controlled heating to 50°C and cooling to $10-14^{\circ}\text{C}$ below ambient for 37mm fluid-filled Petri dish. Supports contact and TappingMode in fluid.. Single point temperature stability is $\pm 0.5^{\circ}\text{C}$ (heating) and $\pm 1.0^{\circ}\text{C}$ (cooling). Overall temperature gradient is $< 2^{\circ}\text{C}$ within the optical viewing area. Includes fluid flow inlet/outlet ports and single gas flow port (0.5 - 2.0 l/min), heated/cooled sample chamber with integral temperature sensor, heater controller with readouts for set point and sample chamber temperatures, two evaporation covers, and separate external temperature sensor and meter for direct monitoring of fluid temperature. Requires fluid cantilever holder (model BFCH) and models DNP or DNP-S or other high temperature fluid cell compatible probes. Model ISBIO-2 acoustic enclosure for environmental temperature stability strongly recommend (required for low-drift AFM imaging). NOTE: Not compatible with the Dimension Closed Loop Scan Head (Model DAFMCL). 	£12,903
8	1	DAFMCL	<p>Dimension Closed-Loop SPM Microscope Head</p> <ul style="list-style-type: none"> SPM/AFM scanner with horizontal imaging area of $90\mu\text{m} \times 90\mu\text{m}$ nominal maximum and a vertical range of $6\mu\text{m}$ nominal maximum. Sensored in X and Y for high accuracy/precision imaging, positioning, zooming, nanomanipulation and nanolithography.. Includes tip holder and TrakScan optical lever position detection system. CE compliant. NOTE: DAFMCL replaces DAFM on the current quotation. 	£32,258

QUOTATION

Veeco Instruments Ltd, Nanotech House, Anderson Road, Buckingway Business Park SWAVESEY, CAMBRIDGE CB4 5UQ
 Phone: 01954 233900
 Fax: 01954 231300

Optional Items (cont)

Item	Qty.	P/N	Description	Price
9	1	BIOFG	Frame Grabber Option for BioScope AFM <ul style="list-style-type: none"> • Video card and vision software for BioScope AFM. • Provides tip and sample viewing in window on NanoScope control monitor. • Allows saving of video images for processing with NanoScope software, printing, or export for presentation and publications. • Available for supported Nikon, Olympus, and Zeiss inverted optical microscopes. • Requires user-supplied supplied CCD camera and cabling. 	£968

EMITECH

EMITECH LTD
 SOUTH STOUR AVENUE
 ASHFORD
 KENT TN23 7RS

TEL: (01233) 646332
 FAX: (01233) 640744
 ENGLAND (44)
 E-Mail: em@emitech.co.uk
 Internet: <http://www.emitech.co.uk>

QUOTATION

TO: Prof. Michael Anderson
 Dept. of Chemistry
 UMIST
 P O Box 88
 Manchester
 M60 1QD

QUOTATION NO. : K2620 - Revised
DATED : 27th June 2003
VALIDITY : **1st April 2004**
DELIVERY : 4-6 Weeks
SUPPLY : 240/115V 50/60Hz.
GUARANTEE : 2 Years

TEL NO.: 0161 200 4517
FAX NO.: 0161 200 4559

CAT.NO.	DESCRIPTION	TOTAL PRICE
EK 3137	K575x Turbo Sputter Coater	£ 10,098.00
	<p>Turbo Molecular Pumping & Peltier Cooled Sputter Head for Ultimate Sputter Performance. For Noble or Oxidising Targets i.e. Chromium/Gold, High Resolution Cool Magnetron Head. Chamber Size: 165mm Dia x 125mm H Base Size: 110mm Dia x 115mm H. Fitted with Chromium Target as Standard. <i>Alternative Target material can be specified, range of other targets available.</i></p>	
	Backing Pump No. 3 Two Stage Approx. 4m ³ /Hr Complete with vacuum Hose. Complete with Coupling Kit & Oil Mist Filter <i>*Optional Diaphragm Pump for Total Oil & Contamination Free System.</i>	£ 995.00
	Less 10% Educational Discount	-£1,109.30
	TOTAL GOODS	£ 9,983.70
	PACKING & DELIVERY	£ 90.00
	NET TOTAL	£10,073.70
	V.A.T. @ 17,5%	<u>£ 1,763.00</u>
	TOTAL GOODS	<u>£11,836.70</u>

**EMITECH QUALITY
 2 YEAR WARRANTY**

ANNEXE 3: Letters from Terasaki and Taulelle



Department of Physical, Inorganic and Structural Chemistry

Professor Osamu TERASAKI

Professor M.W. Anderson
UMIST Centre for Microporous Materials
Department of Chemistry, UMIST
PO Box 88, MANCHESTER M60 1QD
United Kingdom

24th June, 2003.

Dear Mike,

With regard to your application to EPSRC for support for a project concerning crystal growth in open framework materials I am very happy to write this letter. As you know, we have a long standing interest in this field, to which we have been applying electron microscopy techniques to the study of surface structure. This work is demanding but we have developed specific methods to overcome technical difficulties. Microscopy methods are now proving to be extremely important in the study of crystal growth, particularly when combined with AFM. Consequently, a combination of our expertise should lead to a powerful collaboration.

At Stockholm, where I have recently taken up a chair in Structural Chemistry, we are well equipped to study these problems, but owing to time constraints I would also like to work with Dr Viveka Alfredsson from the University of Lund who has special expertise in this area. We would both be very happy to host and supervise a student from Manchester for one year during the course of their PhD studies. This should be sufficient time for them to gain all the necessary expertise to study such problems.

We look forward to a successful collaboration.

Best regards,

A handwritten signature in black ink that reads 'Osamu Terasaki'.

Osamu Terasaki
Professor of Structural Chemistry

Structural Chemistry, Arrhenius Laboratory, Stockholm University, S-106 91 Stockholm, SWEDEN
Phone: +46 8 162379, Fax: +46 8 163118, E-mail: terasaki@struc.su.se <http://www.fos.su.se/struc/>



RMN et Chimie du Solide

Tectonique Moléculaire du Solide

Université Louis Pasteur , UMR 7140 ULP-CNRS
4 Rue Blaise Pascal, 67070 Strasbourg Cedex, France

Dr. Francis Taulelle

Directeur de Recherche CNRS
Tel: 88 41 60 67, Fax: 88 60 75 50
e-mail: taulelle@chimie.u-strasbg.fr

to Pr. M. Anderson
UMIST

Strasbourg june the 25th, 2003

Dear Mike,

With regard to your application to EPSRC for support for a project to study open-framework crystal formation processes *via* a combination of different experimental approaches including AFM, microscopy, NMR, XRD and mass spectrometry, I would be happy to host a PhD student from Manchester for one year in my new location in Versailles.

The student will be based at the Institut Lavoisier. Two types of NMR facility will be in place: a 200 MHz NMR spectrometer dedicated to studying *in-situ* NMR of hydrothermal synthesis; and a 500 MHz wide-bore spectrometer for performing NMR crystallographic determinations. The student will be able to work on both crystallogenesis and nucleation and growth and as the equipment required partly overlaps with your own equipment in Manchester, exchange of students will be very efficient.

My specific contribution for the one year stay of a PhD coming to Versailles is two-fold as follows.

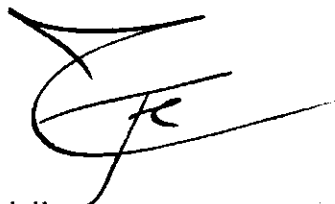
First, we can follow the formation of pre-nucleation building units (PNBUs) by *in-situ* NMR. As zeolites comprise mainly silica-based building units, one may start with 15 to 20% enriched ²⁹Si solution, however with the application of numerical processing methods we shall be able to work at natural abundance levels. The purpose of such studies is to prove the existence of the specific PNBUs that lead to crystal formation and to derive reaction orders from the kinetics of growth. The latter parameter considerably constrains the mechanism of PNBUs inclusion in the crystal. Two dimensional experiments such as INADEQUATE will be performed to get the PNBUs structure and kinetics at low signal to noise ratio using the power of ANAFOR data processing.

Second, we can study the interfacial mechanistic steps of integration of PNBUs onto crystals. NMR crystallographic determination coupled to classical XRD structure determination will help to elucidate the last steps of condensation. This strategy has already been used efficiently for: $\text{AlPO}_4\text{-CJ2}$, ULM3, ULM4, aluminophosphate MIL-74, titaniumfluorophosphates and SAPO-34. Coupled to polycrystalline powder diffraction with *in* and *ex-situ* measurement, NMR crystallographic structure determination greatly facilitates understanding the details of crystal formation.

The *in-situ* work will be supervised on a daily basis by M. Haouas, Chargé de Recherches CNRS who is in charge of the *in-situ* NMR program. The acquisition of crystallographic NMR data will be done with the help of G. Fink, Ingénieur de Recherche CNRS, in charge of the solid-state instrument facility. Software facilities will be provided for both *in-situ* exploitation of data and NMR crystallography. I will have overall supervision of the activities of the aforementioned student during his / her stay in Versailles.

I look forward to a fruitful collaboration.

Best wishes,

A handwritten signature in black ink, appearing to be 'FT' with a large flourish above it.

Francis Taulelle