Group Summary Form

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| Group Code: smw | Number of proposals: 3 |

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| Title of proposed project | **Authors** | **Group code** | Software | Tier1/2 | Work/RDFGb | | TimekAU |
| **Materials Discovery** |  | **discov** |  |  |  | |  |
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| Materials Discovery |  |  |  |  |  |  | **0** |

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| **Biomaterials and Soft Matter** |  | **biosoft** |  |  |  | |  |
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| Biomaterials and Soft Matter |  |  |  |  |  |  | **0** |

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| **Environment and Smart Materials** |  | **enviro** |  |  |  | |  |
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| Environment and Smart Materials |  |  |  |  |  |  | **0** |

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| Energy (Generation, Storage, Transport) |  | **power** |  |  |  | |  |
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| Energy (Generation, Storage, Transport) |  |  |  |  |  |  | **0** |

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| **Fundamentals of Low D Materials** |  | **nano** |  |  |  | |  |
| Analysis of carbon nanowires | D. Deacon-Smith | smw | VASP  KLMC | 1 | 250 | 0 | 12,000 |
| Prediction of TiO2 Clusters | M. Farrow | smw | KLMC  FHI-aims | 1 | 100 | 0 | 2,000 |
| Fundamentals of Low D Materials |  |  |  |  | 300 | 0 | **14,000** |

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| **Reactivity and Catalysis** |  | **react** |  |  |  | |  |
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| Reactivity and Catalysis |  |  |  |  |  |  | **0** |

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| **Fundamentals of Bulk** |  | **bulk** |  |  |  | |  |
| Analysis of defects in KTaO3 | D. Deacon-Smith | smw | VASP  KLMC | 2 | 250 | 0 | 12,000 |
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| Fundamentals of Bulk |  |  |  |  | 200 | 0 | **12,000** |

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| **Fundamentals of Surfaces/ Interfaces** |  | **surfin** |  |  |  | |  |
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| Fundamentals of Surfaces/ Interfaces |  |  |  |  |  |  | **0** |

Group Members who:

|  |  |
| --- | --- |
| will attend the meeting | Scott Woodley, Jane Brown, Daniel Deacon-Smith |
| will not be attending the meeting | Matthew Farrow |
| have recently left (details in Google form) | Sam Johnston, Peter Jones |

NB: in the first table I only ask for expected usage on work and RDF (as home is for software not data), and tier 1 implies ARCGHER and tier 2 implies THOMAS. Please do not use “¶” i.e. “carriage returns” for a new line within a cell in the table as it makes it difficult to cut and paste into an Excel sheet.