

JOB DESCRIPTION

Job Title: Computational Solid-State Scientist

Reports to: Materials Science Team Leader

Salary Band: TBA

SUMMARY OF THE ROLE

The postholder will work within the Research and Innovation team to be responsible for managing the day-to-day administration of the CCDC CSP Blind Test VII and supporting multi-disciplinary CSP initiatives to raise the profile of the CCDC in the CSP community

MAIN DUTIES AND RESPONSIBILITIES

Main responsibilities

- Manage the day-to-day administration of the CCDC CSP Blind Test VII. This will involve:
 - Coordinating with interested parties on shaping the CSP Blind Test
 - Coordinating with partners to acquire suitable test sets for inclusion in the blind test that fulfil the specified test needs
 - Negotiating the participation of experimental groups to generate more information for selected test sets
 - Helping to define the rules for participation
 - Providing entrants with the necessary information at the start of the test
 - Managing the process of accepting entrants for the test subject to any entry requirements in the test specification
 - Fielding any support for the test
- Develop workflows, using off the shelf or new tools, for preparation and post-processing of the test results. This will involve:
 - Development of new tools for assessment of CSP submissions, prototyping these on existing data
 - In-silico preparation of test systems
 - Using the tools to generate reports at the various test stages for each participant and communicating the results back to them
- Finalisation of the Blind Test VII activities, writing papers that outline the test and results, organising and managing meetings for the blind test assessment and dissemination.
- Support the expansion of CSP toolkit & initiatives. This will involve:
 - Testing and validation of existing or newly developed methodologies & approaches

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Quality, Innovation, Passion, Community, Collaboration, Integrity, Customer Centricity, Agility

- Use the developed CSP toolkit for researching functional materials design with key external collaborators
- Dissemination of scientific findings via reports, presentations and peer review publications
- Application of computer-aided approaches to accelerate drug development workflows with key partners. This will involve:
 - Use of computational methods, mostly CSP techniques but not limited to, to better understand drug-like solid form landscapes through informatics-based approaches
 - Supporting the development of new computational tools and workflows
 - Dissemination of scientific findings via reports, presentations and peer review publications
- Undertake additional tasks and responsibilities as may be reasonably expected of the role and as necessary in order to achieve the objectives of the team.

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PERSON SPECIFICATION

Qualifications	
A PhD, or equivalent experience, in the field of Crystal Structure Prediction or solid-state modelling is highly desirable, though consideration will be given to candidates from related fields.	Essential
Experience	
Experience of using initiative to drive forward research ideas	Essential
Experience in the use of computational methods for predicting the structure and relative stability of crystalline materials	Desirable
Autonomy managing IT systems, maintaining code and using scripting language (primarily Python) to develop helper applications. Knowledge of unix/linux will be an advantage	Desirable
Experience of writing scientific papers and summarizing scientific findings concisely and clearly	Desirable
Experience in the use of CSDS data and software	Desirable
Personal Characteristics	
Ability to work independently and with initiative	Essential
Ability to work to deadlines	Essential
Dedicated and self-motivated, keen to learn new skills	Essential
Effective time management	Essential
Excellent written and oral communication skills	Essential
Inquisitive nature, interested in researching and developing crystal structure prediction methods	Essential
Flexible approach to work	Essential

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Good interpersonal skills	Essential
Ability to work in a team	Essential

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