UNIVERSITY OF WARWICK

Job Description

Job Title	Research Fellow in Computational Chemistry
Department	Chemistry
Grade	FA6

Job purpose (a brief summary of the role)	To develop a new computational strategy for catalyst design for CO2 conversion, using a combination of automated reaction discovery, microkinetics, and optimization. To develop improved machine-learning strategies for characterization of chemical reactions, including evaluation of reaction barrier heights and reaction rates. To deploy computational strategies to propose and optimize new catalyst systems to facilitate target chemical transformations of CO2.
Duties and responsibilities	1. To develop robust software capable of optimizing catalysts to enable new chemical transformations of CO2; 2. To engage in high-quality, sustainable and robust software development implementing automated catalyst design strategies; 3. To develop, test and optimize new machine-learning strategies for reaction barrier or reaction rate characterization; 4. To engage in regular progress meetings and individual supervision, and to support junior group members as appropriate; 5. To generate publishable research describing automated catalyst design; 6. To actively engage in the dissemination of research results, including preparation of journal articles and regular attendance and presentations at both national and international academic conferences; 7. To act with professionalism at all times and show respect to their colleagues and to understand and adhere to the University's value of dignity at work; they are also expected to work collegially and to support all the teams with which they have contact in achieving the University's objectives. 8. Any other duties commensurate with the grade and level of responsibility of this post, for which the post holder has the necessary experience and/or training.

Person Specification

The Person Specification focuses on the essential and desirable knowledge, skills, experience and qualifications required to undertake the role effectively. This is measured by (a) Application Form, (b) Test/Exercise, (c) Interview, (d) Presentation.

Essential Criterion No.	Essential Criterion Description	Measured by
E1	A PhD or equivalent in Computational Chemistry.	A
E2	Experience of generating high-quality, robust software for computational chemistry projects.	C & D
E3	Strong working knowledge of AI/ML strategies in computational chemistry.	A,C & D
E4	Good publication track record, appropriate to career stage.	A
E5	Excellent oral and written communication skills.	A,C & D
E6	Working knowledge of typical computational chemistry strategies for reaction analysis, such as minimum-energy path calculations and relevant *ab initio* calculation methods	A,C & D
E7	An ability to work collaboratively and effectively with academic and administrative colleagues, and with colleagues outside the University to promote collegiality.	A & C

Desirable Criterion No.	Desirable Criterion Description	*Measured by*
D1	Knowledge of homogeneous catalysis and mechanistic chemistry.	A & C
D2	Knowledge of state-of-the-art generative AI and optimization strategies for molecular design.	A & C
D3	Experience of supporting junior researchers, such as PhD students or Masters students.	A & C