## JOB DESCRIPTION

**Research Associate**

**Vacancy Ref:** A2630

<table>
<thead>
<tr>
<th>Job Title:</th>
<th>Research Associate</th>
<th>Present Grade: 6</th>
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<tbody>
<tr>
<td><strong>Department/College:</strong></td>
<td>Department of Chemistry</td>
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<td><strong>Directly responsible to:</strong></td>
<td>Andrew Kerridge</td>
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<td><strong>Supervisory responsibility for:</strong></td>
<td>Undergraduate and postgraduate students</td>
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### Other contacts

**Internal:**
Staff and postgraduate students of the Department of Chemistry

**External:**
Helmholtz-Zentrum Dresden-Rossendorf, University of Manchester

### Major Duties:
The postdoctoral research associate will develop a novel computational approach for exploring the electronic structure of heavy element coordination complexes. This will involve the exploitation of the inherent flexibility of the pseudopotential concept. The postdoctoral research associate will be responsible for implementation and testing of this approach, as well as its application to target systems.

### Key Responsibilities

Under the supervision of Dr Andrew Kerridge the postdoctoral research associate will:

- Develop a series of tuneable pseudopotentials for a number of chemical elements across the periodic table
- Perform a range of test simulations on simple halide coordination complexes of f-elements and provide a comprehensive mapping of the character and strength of ion-ligand binding as electronic properties of the ligand and central ion are modified
- Develop models of a range of synthetically relevant ligands, incorporating the electronic effects of standard substituents, via the tuneable pseudopotentials developed
- Perform state of the art simulations of tuned models of relevant f-element complexes
- Develop computational models of novel complexes with predefined properties
- Contribute to the running of the research group
- Prepare internal reports, and progress reports for the funder (Leverhulme Trust)
- Participate in the normal activities of the research group, including meetings and presentations
- Have supervisory responsibility for undergraduate and postgraduate students
- Prepare manuscripts for publication in collaboration with the PI
- Disseminate research findings at national/international meetings and conferences
- Participate in departmental seminars and faculty conferences
- Undertake necessary training and development
- Other duties commensurate with the grade of the post, as directed by the PI