

Postdoctoral Research Fellow position in the area of Computational Catalysis is available at the Department of Chemical and Biomolecular Engineering at the National University of Singapore (#3 in Chemical Engineering according to QS World University Rankings). The position is open for 1 year with a flexible starting date and could be extended depending on mutual interest.

The applicant will work with Prof. Sergey Kozlov in the Computational Nanocatalysis group, which focuses on the simulations of physical and chemical interactions in emerging classes of nanostructured materials. More information about the group can be found at <https://blog.nus.edu.sg/companocat/>. The applicant will use periodic density functional (DFT) simulations and the atomic simulation environment (ASE) to characterize the structure and catalytic activity of nanocomposite catalysts. The research will focus on realistic DFT studies of alloy nanocatalysts with complex structures for CO₂ reduction into valuable multicarbon products performed in collaboration with world-leading experimental teams.

Qualifications:

- Ph.D. in Chemistry, Materials Science, Physics or Chemical Engineering
- Experience in DFT studies of heterogeneous catalysis, electrochemistry, or nanostructured materials using VASP
- The ability to creatively contribute to collaborations with experimental colleagues.
- Excellent writing skills and fluency in English.
- Knowledge of shell scripting and Python.

The applications should be submitted via the following link:
<https://careers.nus.edu.sg/job-invite/13227/>

We will consider all applications containing:

- Cover Letter
- Curriculum Vitae
- Publication List
- Contact details of at least 4 references (including Ph.D. supervisor) willing to provide recommendation letters.
- Additional information may be requested from short-listed candidates.