Postdoctoral position: Atomistic modeling of materials

Postdoctoral position in atomistic modeling of materials is available at the Research Center for Electrochemical Energy Storage of the Skolkovo Institute of Science and Technology, in the group of Prof. Andriy Zhugayevych. The postdoctoral project involve first-principle modeling of materials for energy and optoelectronics, including organic and inorganic semiconductors, cathode/anode materials for metal-ion batteries, conjugated polymers for organic field effect transistors and solar cells etc.

Position is available immediately and is open until filled. Compensation package is locally highly competitive including medical insurance and relocation/housing allowance if applicable. For more information please see http://join.skoltech.ru and contact Andriy Zhugayevych.

Responsibilities

- Perform and supervise basic first-principle calculations within current research projects of the group and Research Center including:
  - Structure and total energies: optimized, PES, MD, statistical, stability
  - Electronic structure: MOs, pDOS, charge/spin density, excited states
  - Spectroscopy: UV-Vis, IR, Raman
  - Electrochemistry: IP/EA, ion intercalation potential, reaction constants
  - Energy/charge transport: transfer and vibronic couplings, ion diffusion barriers
- Sustain and expand computational capabilities for materials modeling including calculation of material properties, modeling of basic processes, screening of materials, keeping materials database, validation of theoretical methodology.
- Communicate results of work in peer-reviewed publications and oral/poster presentations.

Qualifications

- Experience in materials modeling relevant for the position.
- "Hands-on" experience with computational materials science of molecules and solids in LAMMPS, Gaussian, VASP or equivalent set of software packages.
- Proficiency with programming languages and numerical methods used in scientific research, including Python and Maple.
- Ability to work independently and in team, effectively collaborate with both theoreticians and experimentalists.
- Excellent communication and writing skills, as evidenced by publications and cover letter.
- Ph.D. in computational materials science or related field.

Application

To apply, send email to a.zhugayevych@skoltech.ru with "postdoc application" in the subject. Please attach: 1) cover letter including statement of intent, brief description of your relevant qualifications, and names of 2-3 references; 2) CV including publication list; 3) copies of graduate transcripts as a single pdf-file; 4) preprints of three selected publications.

References
- http://crei.skoltech.ru/cee
- www.materialsproject.org; www.molecularspace.org
- Annu Rev Phys Chem 66, 305 (2015); Chem Mater 23, 4032 (2011); etc.