Postdoc position on machine-learning-based interatomic potentials: development and/or applications

There is a postdoctoral researcher position available to work with Dr. Miguel Caro at Aalto University, Finland, on development and applications of machine-larning-based interatomic potentials. The position is for up to four years as part of the Academy of Finland funded COMPEX project. The focus of the project is on improving the accuracy and speed of Gaussian approximation potentials and SOAP many-body descriptors [1,2,3], augmenting structural kernels with electronic structure information [4], training and validating new machine-learning interatomic potentials, and applying these approaches to study the growth of carbon-based nanostructures [5], including long time-scale effects [6]. The successful applicant will be involved in some of these efforts, but not necessarily all of them, depending on their specific background and expertise. This project will feature strong international collaborations with Prof. Gábor Csányi and Dr. Volker Deringer (University of Cambridge) and Prof. Hannes Jónsson (University of Iceland), as well as local collaboration at Aalto.

We are looking for a motivated and talented PhD graduate in Physics, Chemistry, Materials Science, Computer Science, Mathematics, or related areas. Your fields of expertise comprise some of the following topics (familiarity with all of them is not a requirement):

- Density functional theory
- Machine learning (in particular applied to atomic systems) and numerical methods
- Molecular dynamics and force fields
- Transition state theory and long time-scale dynamics
- Code development and high-performance computing

Candidates must be proficient in scientific computing and familiar with programming and/or scripting. A strong command of written and spoken English is essential.

Interested candidates can send their applications and informal enquiries to Miguel Caro (miguel.caro@aalto.fi) in the form of one single PDF file with the following information:

- Motivation statement (max. 1 page)
- Curriculum vitae (max. 2 pages)
- Link to Google Scholar profile (make sure you don't list someone else's publications in it)
- Titles of up to 5 of the publications most representative of your work, with a description of how you were involved in the work (max. 2000 characters per publication)
- Contact information of 2–3 senior academics willing to provide a recommendation upon request

As guideline, the approximate average monthly salary (after tax) for postdoctoral researchers at Aalto University is circa 2600 EUR. Employment includes occupational health care as well as the regular benefits of the Finnish social security system. Finland is routinely ranked among the top countries in the world regarding security, human development, inclusiveness, equality and overall quality of life. Qualifying individuals with all personal backgrounds, including those belonging to minorities underrepresented in the Natural Sciences, are welcomed to apply.

The project will start as soon as September 1st 2019 (this is also the preferred date). Applications will be accepted until the position is filled.

[1] A. P. Bartók, M. C. Payne, R. Kondor, G. Csányi. Phys. Rev. Lett. **104**, 136403 (2010).
[2] A. P. Bartók, R. Kondor, G. Csányi. Phys. Rev. B **87**, 184115 (2013).
[3] M. A. Caro. arXiv:1905.02142 (2019).
[4] M. A. Caro, A. Aarva, V. L. Deringer, G. Csányi, and T. Laurila. Chem. Mater. **30**, 7446 (2018).
[5] M. A. Caro, V. L. Deringer, J. Koskinen, T. Laurila, and G. Csányi. Phys. Rev. Lett. **120**, 166101 (2018).
[6] G. Henkelman and H. Jónsson. J. Chem. Phys. **115**, 9657 (2001).