**Postdoc Position in Atomistic Machine Learning Applications for Sustainable Chemistry at the University of Pittsburgh**

An experienced postdoc is needed to carry out research using quantum chemistry machine learning methods for green chemical design in the University of Pittsburgh's Department of Chemical and Petroleum Engineering in collaboration with Profs. John Keith (R.K. Mellon Faculty Fellow in Energy) and Eric Beckman (Director of the University's Mascaro Center for Sustainable Innovation).

The postdoctoral candidate should have strong programming skills as well as experience in the development and application of artificial neural networks and/or other modern machine learning representations being developed for atomic scale modeling.[1,2] Furthermore, knowledge/experience in one or more of the following fields is desirable:

- Organic, inorganic, and/or biological chemistry and/or chemical physics
- Computational quantum chemistry calculations of ion solvation energies and/or molecular p$K_a$s
- Modeling aqueous environments using polarizable forcefields and/or QM/MM methods
- Quantitative Structure Activity Relationship (QSAR) methods

The candidate should have completed (or should soon complete) a Ph.D. The ideal candidate has a demonstrated record of independently designing and conducting research and publishing results in competitive conferences and journals. The postdoctoral position is intended to serve as a platform to help the postdoc to:

(i) strengthen and develop a research profile through scientific publications and patents
(ii) build a knowledge base for her/his own future research group and/or future entrepreneurship in sustainability engineering
(iii) become a contributor to the development of the widely used Avogadro code[3]

Interested applicants should submit a single PDF file containing: (1) a 1-page cover letter, (2) a CV that includes a list of scientific publications, and (3) the names and contact information for three references.

Pittsburgh is one of the most livable cities in the U.S., and academic research is highly collaborative. For more information about Pittsburgh see: https://www.visitpittsburgh.com. Any questions about this position should be directed to Prof. John Keith (jakeith[at]pitt.edu).

Please apply to the above email address by March 15th, 2018.

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[1] Jörg Behler and Michele Parrinello, *Phys. Rev. Lett.* 2007, *98*, 146401.
[2] Matthias Rupp, Alexandre Tkatchenko, Klaus-Robert Müller, and O. Anatole von Lilienfeld, *Phys. Rev. Lett.* 2012, *108*, 058301.
[3] Marcus D Hanwell, Donald E Curtis, David C Lonie, Tim Vandermeersch, Eva Zurek, and Geoffrey R Hutchison, *J. Cheminform.* 2012, *4*, 17.