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Postdoctoral *ab-initio* position at BOSCH Corporate Research Energy Technologies group

The **Robert Bosch Research and Technology Center North America** is looking for outstanding researchers in the field of **ab-initio computational modeling of materials for energy applications**.
The position is located in our Cambridge, MA office, across from the MIT campus. The position will augment both ongoing internal research efforts within the company and external collaborations within the projects Bosch is supporting as a member of the MIT Energy Initiative. The focus will be on ab-initio modeling of new functional materials, aiming to gain insights into microscopic mechanisms and properties, and to provide guidance for designing new materials for energy conversion and storage applications.

Topics include:

- **Thermoelectric materials**: Focus will be on developing models and applying state-of-the-art first-principles techniques to understand and improve electronic and thermal transport properties.
- **Li-ion batteries:** Thermodynamic and electrochemical properties of materials for high-energy-density storage materials. Emphasis is on computing chemical and thermal stability and optimizing ionic and electronic transport.
- **Photovoltaic** devices: Computational analysis of optical properties, defect energetics and modeling of electronic transport across heterogeneous interfaces.

We are looking for exceptional candidates to interact in a global, dynamic environment that brings together researchers from Bosch in North America, Europe and leading scientists at MIT. Specialized knowledge and skills desired:
- Established research record and several years of experience
- Expertise in ab-initio methods and molecular dynamics
    - DFPT, DFT+U, CPMD, NEB, KMC, GW
    - Extensive experience with modern ab-initio tools (Quantum Espresso, VASP)
- Knowledge of solid-state theory, chemistry and thermodynamics
    - Electron transport, excitations (e.g. electron-phonon coupling), alloy theory
- Solid programming, scripting and data management skills in Linux environment

Computations will be performed at Bosch on in-house cluster machines, with close connection to experiments.

Initial contract is for one year, and is extendible and upgradeable. Compensation and benefits are commensurate with a starting full-time position.

Please send a CV and references to: **33879-CS-1523@boschresearch.hrmdirect.com**

The Bosch Group *is a leading global supplier of technology and services. In the areas of automotive and industrial technology, consumer goods, and building technology, some 272,000 associates generated sales of over 46 billion euros (over $63 billion) in fiscal 2007. The privately owned Bosch Group comprises Robert Bosch GmbH and its roughly 300 subsidiary and regional companies in over 50 countries.* ***Corporate Research*** *at Bosch employs some 1300 researchers at locations in Germany, United States, Singapore, China, Japan and Russia. The effort is part of Bosch's commitment to advancing technology, manifested in 29,000 associates working in research and development units, and total 2007 R&D expenditures of over $5B (7.7% of sales). In accordance to its motto, "invented for life", Bosch is dedicated to responsible use of our environment, and is currently active in renewable energy generation through its photovoltaics business, Bosch Ersol, and energy storage thru its Li-ion battery joint venture, SB LiMotive. To learn more please visit http://www.bosch.us and http://www.boschresearch.com.*

For a small sample of the flavor of ab-initio activities in our North American offices, see:

[1] B. Kozinsky and N. Marzari, "Static Dielectric Properties of Carbon Nanotubes from First Principles", Phys. Rev. Lett. 96, 166801 (2006).

[2] I. Dabo, B. Kozinsky, N. Singh-Miller, N. Marzari, "Electrostatics in periodic boundary conditions and real-space corrections", Phys. Rev. B 77, 115139 (2008).

[3] D. Wee, B. Kozinsky, M. Fornari, N. Marzari, "Direct and Indirect Effects of Filling on Band Structure and Phonon Dispersion of Skutterudites", MRS proceedings, Spring 2009.

[4] S. Petrosyan, M. Fornari, B. Kozinsky, N.Marzari, G. Ceder, "Local ordering and structural instabilities in (Na,Bi)TiO3 perovskites", APS meeting, March 2009.