THE STATE UNIVERSITY OF NEW JERSEY
RUTGERS

Department of Physics and Astronomy • Rutgers, The State University of New Jersey
136 Frelinghuysen Road • Piscataway, NJ 08854-8019

David Vanderbilt
dhv@physics.rutgers.edu • http://www.physics.rutgers.edu/~dhv
Phone:(732) 445-2514 • FAX: 732/445-4400

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Executive Officer
Fellowship Program
The American Physical Society
One Physics Ellipse
College Park, MD 20740-3844

Dear Fellowship Committee,

It is my pleasure to nominate **Karin Rabe** for election as a fellow of the American Physical Society in the Division of Materials Physics. Rabe has an international reputation of the first order as a world leader in the theoretical understanding of structural phase transitions in crystalline solids. In particular, Rabe has made fundamental contributions to the application of first-principles electronic-structure methods to the study of structural phase transitions, especially in ferroelectric and martensitic systems.

The study of structural phase transitions is made difficult by the large length scales involved, so that in most cases direct simulation by ab-initio molecular dynamics is still far from practical. Instead, the most successful work has been based on the "effective Hamiltonian" approach pioneered by Rabe. In this approach, one first identifies the most important low-energy structural degrees of freedom and expands the total energy of the system in terms of these variables, then determines the coefficients of the expansion from first-principles calculations, and finally uses Monte-Carlo or molecular-dynamics simulations to study the thermodynamic properties as a function of temperature.

Rabe's thesis work demonstrating this approach was a *tour de force*, requiring mastery both of modern techniques of statistical mechanics and of *ab-initio* calculations of structural energies to arrive at a first-principles description of the structural phase transitions in GeTe. Her early publications on this are classic works that set the standard for all subsequent work in this field.

Rabe then went through an interlude, as a postdoc at Bell and then upon first arriving at Yale, where she made substantial contributions to the theory of high-temperature superconductors, quasicrystals, and fullerenes. This work served to broaden her interests and expertise, but in retrospect is not very closely coupled to her previous or subsequent work.

In the last decade, first at Yale and then very recently at Rutgers, Rabe has returned to the theme of effective-Hamiltonian methods applied to structural phase transitions, this time with the man application being to ferroelectric perovskites such as $BaTiO_3$ and $KNbO_3$. (Actually, the $BaTiO_3$ work was done in collaboration with my postdoc Zhong and myself, but Rabe took the lead in the conceptual formulation and execution of the effective-Hamiltonian approach.) The perovskites had been a model system for the study of ferroelectricity for decades, and have recently enjoyed widespread renewed attention for a range of possible applications. Despite this, a first-principles atomistic theory of these materials with real predictive power did not previously exist. Thus, her work showing that the effective-Hamiltonian approach could yield a correct description of the complicated phase transition sequences in this class of materials has had a very big impact, as have her subsequent applications of these techniques (and of the machinery of linear-response lattice-dynamical calculations) to elucidated important aspects of the local structure of ferroelectric crystals and alloys – and most recently, of ferroelectric thin-film and superlattice structures. Rabe is also making important contributions to the theory of structural phase transitions in intermetallic compounds such as NbN, Al_2Ru, Ni_2MnGa, and NiTi. Altogether, this work has established her international reputation as perhaps the leading expert in the computational theory of structural phase transitions in solids.

In view of the above, I think it is especially appropriate that Rabe be elected to APS fellowship under the auspices of the DMP. In fact, one of the things that impresses me about her outstanding record of invited talks is that many of these are at conferences on subjects (e.g., ceramics, ferroelectrics, crystallography) which may not have very high visibility to the theoretical condensed-matter physics community at large, but which are on the real "cutting edge" of materials physics.

Rabe is a highly successful and sought-after teacher, and has an unusually strong record of active service to the profession. In connection with the APS Fellowship it may be noteworthy that she served a three year term (1994-1997) as a member-at-large of the Executive Committee of the Division of Computational Physics of the APS. She has been a frequent organizer of conferences and workshops, and recently served a one-year term as Scientific Secretary at the Aspen Center for Physics.

In summary, I am fully convinced that Rabe meets the criteria for Fellowship in the American Physical Society, and I recommend her election to this Fellowship in the strongest possible terms.

Sincerely,

David Vanderbilt
Professor of Physics