Citation

For fundamental contributions to the development and application of theoretical and computational methods for the study of structural phase transitions in solids.

Supporting paragraph

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. In most such cases, direct simulation by ab-initio molecular dynamics is still far from practical, and 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 was the first to demonstrate such an approach in her early work on GeTe. However, the biggest impact has followed from her application of this approach to ferroelectric perovskites such as $BaTiO_3$ and $KNbO_3$, where the approach was shown to yield a correct description of the complicated phase transition sequences in this class of materials. Most recently her work has elucidated important aspects of the local structure of ferroelectric alloys and, especially, of ferroelectric thin-film and superlattice structures. Her work on structural phases and phase transitions in intermetallic compounds has also had a major impact, and in addition she has made significant contributions to the theory of high-T_c superconductors, quasicrystals, and fullerites.