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Linking Quantum and Classical Descriptions: Hierarchical Development of Born-Oppenheimer-like Approximations YING HU, Department of Physics and Astronomy, Vanderbilt University — The Born-Oppenheimer (BO) approximation is ubiquitous in quantum mechanical calculations of molecular wavefunctions. Here I report an extension of traditional BO approximation to a hierarchy of BO-like approximations which enables dynamic linking among distinct scales in complex crystals, from the quantum world to the macroscopic. At first, the usual BO approximation allows us to average out electrons to give descriptions of slow motion of nuclei. Then we describe an atom in crystals with two classes of independent variables corresponding to two distinct time scales: lattice deformation and relative atomic motion. We invoke a BO-like Ansatz as constraint to construct a "constrained distribution function" so that phonons are averaged out from lattice deformation. To progress further, we use BO-like approximation to modify constraints so as to account for defects. The BO-like approximations is further extended from separating distinct time scales to different length scales. The ultimate hierarchy of BO-like approximations enables formulation of nonequilibrium multiscale statistical mechanics where electrons, phonons, defects and lattice deformation are dynamically coupled.

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