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Quantum Mechanics Based Multiscale Modeling of Materials[1]

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We present two quantum mechanics based multiscale approaches that can simulate extended defects in metals accurately and efficiently. The first approach (QCDFT) can treat multimillion atoms effectively via density functional theory (DFT). The method is an extension of the original quasicontinuum approach with DFT as its sole energetic formulation. The second method (QM/MM) has to do with quantum mechanics/molecular mechanics coupling based on the constrained density functional theory, which provides an exact framework for a self-consistent quantum mechanical embedding. Several important materials problems will be addressed using the multiscale modeling approaches, including hydrogen-assisted cracking in Al, magnetism-controlled dislocation properties in Fe and Si pipe diffusion along Al dislocation core.

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