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First-principles AFM image simulation with frozen density embedding theory[1] YUKI SAKAI, ALEX J. LEE, JAMES R. CHELIKOWSKY, Univ of Texas, Austin — We present efficient first-principles method of non-contact atomic force microscopy (nc-AFM). Ordinary nc-AFM simulations based on density functional theory (DFT) require exhaustive computational cost because it involves thousands of total energy calculations. Regarding the sample as a fixed external potential can reduce the computational cost, and we adopt frozen density embedding theory (FDET) for this purpose. Simulated nc-AFM images with FDET using a carbon monoxide tip well reproduces the full DFT images of benzene, pentacene, and graphene, although optimized tip-sample distances and interaction energies in FDET are underestimated and overestimated, respectively. The FDET-based simulation method is promising for AFM image simulation of surfaces and two-dimensional materials.

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