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Adaptive molecular dynamics for long time-scale simulations[1]
YUKI SAKAI, JAMES R. CHELIKOWSKY, University of Texas at Austin — We propose an adaptive molecular dynamics method that combines classical and first-principles Born-Oppenheimer molecular dynamics. In this adaptive method, classical and Born-Oppenheimer dynamics are performed sequentially and alternately. The parameters of classical model potentials are fitted by using a force-matching method every time after the Born-Oppenheimer molecular dynamics. This method reduces the heavy computational load of the Born-Oppenheimer dynamics while the update of model potential parameters enable one to incorporate the change in bond order and coordination number. By using the current method, we can qualitatively reproduce the power spectra of organic molecules obtained with Born-Oppenheimer molecular dynamics. We also discuss the computational speed up and stability of this method.

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