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The Road to Interoperable Simulation Software: Examples Using the Qbox Code[1]

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The diversity of available simulation software implementing various methods–from atomistic classical molecular dynamics to quantum many-body perturbation theory–makes it highly desirable to couple these codes in a seamless fashion. We discuss the approach taken with the Qbox code to couple first-principles molecular dynamics with advanced sampling algorithms and with GW electronic structure calculations.
http://qboxcode.org
http://www.quantum-simulation.org

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