

another code

From: Shakib, Farnaz (farnaz.a.shakib@njit.edu)

To: sandrabrown92821@yahoo.com

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Hi Sandra,

Sorry, the previous MQCL code that I sent you includes only one classical coordinate, 1 collective solvent coordinate that is coupled to PCET. In the attached source code, we have also a bath of classical harmonic oscillators. You can see the force.f90 which calculates the classical forces, as well as runnve.f90 that runs velocity-Verlet algorithm. The corresponding paper is attached as well.

Also, in the PCET_model that I sent you, I have added comments to the kinetic.f90 in the kinetic folder.

Thanks,
Farnaz

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