PCET and MQCL codes

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To: sandrabrown92821@yahoo.com

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Hi Sandra,

I hope all is well. I apologize for the delay in sending you the codes.

The model is described in the paper attached. What we did was to separate all the quantum mechanical (related to the coordinates of proton and electron, qp and qe) and classical (Q) parts of the Hamiltonian. Then, we integrated the quantum mechanical part beforehand <Psi|H|Psi> where we expanded Psi in terms of 25 harmonic oscillators for proton and 25 oscillators for electron. In the attached folder, the PCET_model contains all these integrations in separate files for kinetic energy, potential energy, coupling energy, and overlap of the wavefunction. After running integration and creating output files in each directory I used to run a small code (reorder.f90) to write them in terms of indices of a 625 by 625 matrix. Then there is a matrix.f90 code to write all these elements in a matrix.in file which will be read in the main code and the classical parts will be added there. Then, the whole matrix will be diagonalized at every time step.

I have also attached the MQCL code but I don't think you need it. The only part related to the model is concerted_PCET_momentum4/src/adiab_nve.f90 where we read in the matrix.in and build the whole model.

Honestly, I am not sure if these will help you at all. Please take a look at the paper and the model and let me know if we need to meet and discuss.

Thanks,
Farnaz

For_Sandra.zip

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