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Quantum Monte Carlo study of water-acene systems[1] JIAWEI XU, RICHARD CHRISTIE, KENNETH JORDAN, University of Pittsburgh — Electronic structure quantum Monte Carlo methods are used to calculate the energies of a water molecule interacting with benzene, anthracene, and coronene. Localized orbitals represented as spline functions are used to reduce the computational cost of the calculations for larger water-acene complexes. The prospects of using this approach to determine the interaction energy between water and graphite is discussed.

[1]NSF

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