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Diffusion Monte Carlo characterization of a methane molecule in a $(H_2O)_{20}$ dodecahedral cage[1] KENNETH JORDAN, MICHAEL DEIBLE, University of Pittsburgh — The diffusion Monte Carlo method is used to investigate the interaction of a water molecule with a dodecahedral $(H_2O)_{20}$ cage as found in the methane hydrate crystal. The DMC value of the interaction energy between the methane molecule and the cage are compared with the results of MP2 and symmetry-adapted perturbation theory (SAPT) calculations [1]. In addition, the net interaction energy is decomposed into two- and three-, and $n \geq$ four-body contributions. The two- and three-body contributions are further analyzed in terms of SAPT calculations [1,2].

[1] A. J. Misquitta, R. Podeszwa, B. Jeziorski, and K. Szalewicz, J. Chem. Phys. **123**, 214103 (2005); A. Hesselmann, G. Jansen, and M. Schütz, J. Chem. Phys., **122**, 014103 (2005).
[2] R. Podeszwa and K. Szalewicz, J. Chem. Phys., **126**, 194101 (2007).

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Kenneth Jordan
University of Pittsburgh

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