A NEW POTENTIAL ENERGY SURFACE FOR H_2–N_2O AND PIMC SIMULATION PROBING SUPERFLUIDITY AND VIBRATIONAL FREQUENCY SHIFTS IN DOPED $para$-H_2 CLUSTERS

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The existence of superfluidity of $para$-hydrogen clusters doped by the linear molecules[a,b,c] such as CO, CO_2 and OCS stimulated our theoretical study of ($para$-H_2)$_N$–N_2O clusters. A new 6D $ab\ initio$ PES for the H_2–N_2O dimer which explicitly included the symmetric and asymmetric vibrational coordinates Q_1 and Q_3 of N_2O was constructed. Four-dimensional global intermolecular PESs were then obtained by fitting the vibrational averaged interactions energies for ν_3(N_2O)=0 and 1 to the Morse/Long Range(MLR) analytical form with theoretically fixed long-range parameters. Using the adiabatic hindered-rotor approximation, effective two-dimensional PESs for the $para$-H_2–N_2O dimer were then generated. Predictions of the infrared spectra of $para$-H_2–N_2O based on these PESs have been in good agreement with the experimental observations.[d] Based on these surfaces, predictions of structural properties, vibrational band origin shifts, rotational dynamics and superfluidity of ($para$-H_2)$_N$–N_2O clusters have been generated using bosonic PIMC simulation methods. The evolution of the calculated shifts agreed reasonably with that for the experimental observations.[e] Reduction of the effective moment of inertia is predicted to occur when the dopant is partially surrounded by the $para$-H_2 solvent, which marked the onset of molecular superfluidity in $para$-H_2. Results obtained using our surfaces and PIMC algorithm will be presented.

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