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Finite Temperature Properties of Clusters by Replica Exchange Metadynamics: The Water Nonamer YINGTENG ZHAI, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China, ALESSANDRO LAIO, ERIO TOSATTI, International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China — We introduce an approach for the accurate calculation of thermal properties of classical nanoclusters. Based on a recently developed enhanced sampling technique, replica exchange metadynamics, the method yields the true free energy of each relevant cluster structure, directly sampling its basin and measuring its occupancy in full equilibrium. All entropy sources, whether vibrational, rotational anharmonic and especially configurational – the latter often forgotten in many cluster studies – are automatically included. For the present demonstration we choose the water nonamer $(H_2O)_9$, an extremely simple cluster which nonetheless displays a sufficient complexity and interesting physics in its relevant structure spectrum. Within a standard TIP4P potential description of water, we find that the nonamer second relevant structure possesses a higher configurational entropy than the first, so that the two free energies surprisingly cross for increasing temperature.

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