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Molecular Dynamics with Quantum Statistics

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Recent experiments on the behaviour of solute species embedded in helium nano-droplets have allowed scientists to address several fascinating questions such as the dynamics of free rotation related to microscopic superfluidity, phenomena of self-assembly, and the shell structure of quantum solvation. From a theoretical point of view, these many-body systems represent a great challenge because of their size and the fact dynamical as well as statistical (helium atoms are bosons) quantum dynamical effects must be accounted for in order to properly describe the observed phenomena. We present a theoretical formalism amenable to the large-scale computer simulation of these systems. Recent results on helium clusters consisting in a few hundred atoms will be discussed

Pierre-Nicholas Roy received his bachelor degree in chemistry from McGill University in 1990. He then pursued graduate studies in theoretical chemistry at Université de Montréal where he received his M.Sc. in 1993 and his Ph.D. in 1997. He spent the year 1997 at the James Franck Institute of the University of Chicago as a Research Associate. He then moved to the University of Utah in 1998 as a Postdoctoral Fellow in the Henry Eyring Institute for Theoretical Chemistry. He returned to Canada to join the University of Alberta where he has been an Assistant Professor of chemistry since 1999. In the year 2000, Pierre-Nicholas Roy has received the Research Innovation Award from the Research Corporation and a New Opportunity Award from the Canada Foundation for Innovation. His group is involved in the development of new computational methods to simulate the dynamics of complex molecular systems.