Séminaire du Pr. Ludwik Adamowicz de l'Université d'Arizona

Titre : Chemical and physical properties of molecules in strong magnetic fields. Non-Born-Oppenheimer calculations with explicitly correlated Gaussian functions.

Résumé : Explicitly correlated all-particle Gaussian functions with shifted centers (ECGs) are implemented within the effective variational non Born- Oppenheimer method introduced ealier by our group to calculate bound states of molecular systems in strong magnetic fields. The Hamiltonian used in the calculations is obtained by subtracting the operator representing the kinetic energy of the center-of-mass motion from the total laboratory-frame Hamiltonian. The calculations reveal some interesting effects related to the structures and spectra of the systems, that may alter the system's chemical and physical behavior.