SEMINAIRE ISMO

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Quantum Chemistry and its role in dynamical studies in ultra-cold collisions

The structure and properties of molecules and their cations plays a fundamental role in a range of dynamical studies such as; ultra-cold collisions, laser cooling and trapping, dissociative electron attachment, dissociative recombination, electron scattering, photoionization and ultrafast dynamics. Ultra-cold hybrid ion-atom traps offer the possibility of microscopic manipulation of quantum coherence in the gas using the ion as a probe. The inelastic processes, particularly charge transfer, may play a significant role in the process of ion loss and is of current interest experimentally. The study of ultra-cold molecules tightly trapped in an optical lattice can expand the frontier of precision measurements and spectroscopy and lead to a deeper insight into molecular and fundamental physics. The interpretation of experimental results requires detailed information on the structure, properties and dynamics and is a prime example where quantum chemistry plays a fundamental role. Electron-density distributions, transition dipole moments and potential-energy surfaces are important for predicting the physical properties and chemical reactivity of molecular systems. Methods used to obtain the structure and dynamics of molecular systems for a variety of molecular complexes will be outlined. The fundamental role played by quantum chemistry in these investigations will be discussed for cross sections and rate coefficients evaluation, for radiative loss, association and charge transfer for a variety of diatomic complexes; $NaCa^+$, HeC^+, CH^+, CH, SiO, CS and C_2. The $NaCa^+$ cation is of current interest to the efforts (experimental and theoretical) of the University of Connecticut group.

Lundi 29 avril 2019 à 11 h

Amphithéâtre du bât 520 (3ème étage)
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