Séminaire GSMA

Nonadiabatic corrections to vibrational levels through core-valence separation of motions in molecules

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1.12.2010-31.01.2011, bât 6, salle D1-106

Abstract

A semi-empirical separation of movements of cores and valence electrons in a molecule is performed, generating coupled equations for the movement of the cores. Far from critical points of the potential energy surfaces, both adiabatic and nonadiabatic corrections turn dependent just on the valence wavefunction. The procedure of evaluating nonadiabatic corrections by replacing the nuclear reduced mass by another one lying between the nuclear and the atomic reduced mass is then justified. A formula for effective core masses based on electron atomic populations is introduced. Nonadiabatic corrections to vibrational levels of H_2 compares very well to the exact results. Corrections to vibrational levels of LiH are then reported and an application to H_3^+ is devised.

Lieu: Salle de réunion du GSMA, bât 6, D1 - 069
Date: 08 décembre 2010 , 11:00 h
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