Electronic Structure and Dynamics in a Strong Magnetic Field

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Strong magnetic fields which compete with the Coulombic forces in atoms and molecules affect structure, energetics, degeneracies, symmetries and dynamics of both the electrons and the nuclei. The complex and coupled nature of the interactions make it difficult to intuitively understand the response of the system to the external field. A direct non-perturbative solution of the system and field is thus undertaken. The findings from the electronic structure study are presented and preliminary investigations of the nuclear dynamics in the strong magnetic field and related challenges are discussed. Hindrances to selective vibrational modes and rotational modes along with field induced couplings completely change the ro-vibrational spectrum.