

Berry phase calculation of the rotational and pseudorotational g-factor in molecules and solids

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The net orbital magnetic moment due to ion rotation or pseudorotation in a molecule or a solid is calculated using standard density functional plane wave methods. The problem addressed here is that while the electrons basically do not influence the mechanical moment of the molecule, they nonetheless do reduce significantly the orbital magnetic moment produced by nuclear rotation (magnetic screening) by a generally unknown amount. This is calculated by assuming an external magnetic field, evaluating the electronic Berry connection resulting from adiabatic ionic evolution, and subtracting that away as a screening term from the magnetic vector potential seen by the bare ions. This method, as well as alternative localized orbital calculations including the magnetic field through a heuristic Peierls phase factor, are tested and found quantitatively accurate for the simplest molecules, H_2^+ , H_2 , whose orbital g-factor has long been known; C_2H_2 and CF_4 , where the orbital g-factor is found respectively marginally positive and marginally negative, in agreement with experiments. Application to pseudorotations is exemplified in benzene and fully employed in the calculation of the screening of soft-mode in incipient ferroelectric perovskites (KTaO_3 and SrTiO_3).