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Electron corrected Lorentz forces in solids and molecules in magnetic field DAVIDE CERESOLI, RICCARDO MARCHETTI, SISSA and DEMOCRITOS, ERIO TOSATTI, SISSA, DEMOCRITOS and ICTP — We describe the effective Lorentz forces on the ions of a generic insulating system in a magnetic field, in the context of Born-Oppenheimer ab-initio molecular dynamics. The force on each ion includes an important contribution of electronic origin, which depends explicitly on the velocity of all other ions, and is given in terms of a Berry curvature, directly suitable for classical dynamics simulations. The formulation is valid at strong magnetic field, where a scheme for ab-initio simulations based on plane wave methods is outlined. As a simple analytical demonstration we present the dynamics of an H_2 molecule in a weak field, describing the electrons approximately through Slater's variational wavefunction.

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