Ab initio study of polar molecules in an optical lattice

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The emerging field of trapping ultracold polar molecules in an optical lattice opens prospects for new physics, chemistry, and quantum computations. The ultimate goal of our study is to provide information needed to achieve control at the quantum level over internal and external degrees of freedom of a polar molecule in an optical lattice. Here we report data concerning polar RbCs molecules. This data includes relativistic electronic potentials, permanent and transition dipole moments, the ground-state molecular dynamic polarizability as function of the internuclear separation, and Franck-Condon factors between vibrational levels of ground and excited states, which are needed to design an optimal optical lattice. We also study interactions between polar RbCs molecules confined in different lattice sites. Theoretical tools include the relativistic multiconfiguration valence bond method for the electronic structure and a discrete variable representation method for the vibrational motion.

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