Ground state properties of alkali and alkaline-earth hydrides

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The ground state potential energy curves of alkali (LiH to CsH) and alkaline-earth monohydrides (BeH to BaH) have been calculated. A pseudopotential formalism including a core-polarization potential has been used. For the valence correlation energy, two different methods, the local spin-density functional and the configuration interaction with single and double excitations, have been employed. Dissociation energies, bond lengths, vibrational frequencies, anharmonicity constants, and dipole moments are reported. The agreement with experimental values, where available, is very good. A discussion and a comparison with other theoretical values, at different levels of approximation, are also included.