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State of the art for ab initio vs empirical potentials for HeH^+ ($2e^-$), BeH^+ ($4e^-$), BeH ($5e^-$), Li_2 ($6e^-$) and BH ($6e^-$) NIKE DATTANI, Kyoto University — For large internuclear distances, the potential energy between two atoms is known analytically, based on constants that are calculated from atomic *ab initio* rather than molecular *ab initio*. This analytic form can be built into models for molecular potentials that are fitted to spectroscopic data. Such empirical potentials constitute the most accurate molecular potentials known. For HeH^+, and BeH^+, the long-range form of the potential is based only on the polarizabilities for He and H respectively, for which we have included up to 4th order QED corrections. For BeH, the best ab initio potential matches all but one observed vibrational spacing to ¡ 1 cm^- accuracy, and for Li_2 the discrepancy in the spacings is ¡ 0.08 cm^{-1} for all vibrational levels. But experimental methods such as photoassociation require the absolute energies, not spacings, and these are still several in several cm^{-1} disagreement. So empirical potentials are still the only reliable way to predict energies for few-electron systems. We also give predictions for various unobserved "halo nucleonic molecules" containing the "halo" isotopes: ^{6,8}He, ^{11}Li, ^{11,14}Be and ^{8,17,19}B.

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