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Accurate Binding Energy of Ytterbium Dimer from Ab Initio Calculations and Ultracold Photoassociation Spectroscopy

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Abstract : Recent proposals to use Yb dimer as an optical clock and as a sensor for non-Newtonian gravity imply the knowledge of its interaction potential. Here, the ground-state Born-Oppenheimer Yb_2 potential energy curve is represented by a semi-analytical function, consisting of short- and long-range contributions. For the former, the systematic ab initio all-electron exact 2-component scalar-relativistic CCSD(T) calculations are carried out. Special care is taken to saturate diffuse basis set component with the atom- and bond-centered primitives and reach the complete basis set limit through n = D, T, Q sequence of the correlation-consistent polarized n-zeta basis sets. Similar approaches are used to the long-range dipole and quadrupole dispersion terms by implementing the CCSD(3) polarization propagator method for dynamic polarizabilities. Dispersion coefficients are then computed through Casimir-Polder integration. The semiclassical constraint on the number of the bound vibrational levels known for the ^{174}Yb isotope is used to scale the potential function. The scaling, based on the most accurate ab initio results, bounds the interaction energy of two Yb atoms within the narrow 734 ± 4 cm^{-1} range, in reasonable agreement with the previous ab initio-based estimations. The resulting potentials can be used as the reference for more sophisticated models that go beyond the Born-Oppenheimer approximation and provide the means of their uncertainty estimations. The work is supported by Russian Science Foundation grant # 17-13-01466.

Keywords : ab initio coupled cluster methods, interaction potential, semi-analytical function, ytterbium dimer
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