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 Yb₂ potential energy curve is represented by a semi-analytical function, consisting of short- and long-range contributions. For the former, the systematic ab initio allelectron 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 ¹⁷⁴Yb 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 \pm 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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