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Long Range Interactions of Ytterbium in Mixed Quantum Gases

CHARLES W. CLARK, JQI, NIST and the University of Maryland, S.G. PORSEV, University of Delaware and PNPI, M.S. SAFRONOVA, University of Delaware, A. DEREVIANKO, University of Nevada, Reno — A first-principles relativistic method is developed for an accurate calculation of the van der Waals coefficients of dimers involving excited state atoms with strong decay channel to the ground state. Accurate values of long-range interaction parameters are needed for efficient production, cooling, and control of molecules. We used the developed methodology to calculate a number of C_6 and C_8 coefficients for Yb-Yb, Yb-Rb, and Yb-Li dimers which are of particular interest for development of optical lattice clocks, studies of fundamental symmetries and quantum gas mixtures, and practical realization of quantum simulation proposals. Our calculations include C_6 coefficients for the Yb–Yb $^1S_0 + {}^3P^o_{0,1}$ and $^3P^o_0 + {}^3P^o_0$ dimers, C_8 coefficients for the $^1S_0 + {}^1S_0$ and $^1S_0 + {}^3P^o_1$ dimers, C_6 coefficients for the Yb–Rb $^3P^o_1 + 5s\,{}^2S_{1/2}$ and $^1S_0 + 5p\,{}^2P^o_{1/2}$ dimers, and the C_8 coefficients for the Yb–Li $^1S_0 + 2s\,{}^2S_{1/2}$ and Yb–Rb $^1S_0 + 5s\,{}^2S_{1/2}$ dimers. We performed detailed uncertainty analysis and provided stringent bounds on all quantities obtained in this work to allow future benchmark tests of experimental methodologies and theoretical molecular models.

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