

Theoretical studies of interatomic forces and atomic properties



HEAD:

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GROUP MEMBERS:

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RESEARCH PROFILE:

Development of quantum theory of atomic properties and interatomic interactions and applications of this theory to metrology and high-resolution molecular spectroscopy.

CURRENT RESEARCH ACTIVITIES:

Development of methods to include relativistic and quantum electrodynamics effects in calculations of atomic properties and interatomic interaction energies. Developments of methods to include the effects of the coupling of electronic and nuclear motion in calculations of interatomic potentials. Development of new perturbation theory techniques for accurate determination of interatomic potentials. Development of new accurate methods of the electronic structure theory. Accurate calculations of electric and refractive properties of atomic gases for applications in metrology.

SELECTED PUBLICATIONS:

1. M. Lesiuk, B. Jeziorski, Size consistency and counterpoise correction in explicitly correlated calculations of interaction energies and interaction-induced properties, *Phys. Rev. A.* 99 (2019) 032712-1 - 032712-10.
2. M. Przybytek, W. Cencek, B. Jeziorski, K. Szalewicz, Pair potential with submillikelvin uncertainties and nonadiabatic treatment of the halo state of helium dimer, *Phys. Rev. Lett.* 119 (2017) 123401-1 - 123401-6.
3. P. Gniewek, B. Jeziorski, Determination of the exchange interaction energy from the polarization expansion of the wave function, *Phys. Rev. A.* 94 (2016) 042708-1 - 042708-6.
4. K. Piszczatowski, M. Puchalski, J. Komasa, B. Jeziorski, K. Szalewicz, Frequency-dependent polarizability of helium including relativistic effects with nuclear recoil terms, *Phys. Rev. Lett.* 114 (2015) 173004-1 - 173004-5.
5. P. Gniewek, B. Jeziorski, Exchange splitting of the interaction energy and the multipole expansion of the wave function, *J. Chem. Phys.* 143 (2015) 154106-1 - 154106-10.