Theoretical study of the rare gases dimers

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The rare gas clusters represent a typical example of van der Waals systems which unusual properties have recently attracted a lot of attention of many researchers. In fact, the development of the technology gives a possibility to study ultracold gases with fully controlled interatomic interaction and to find some universal correlations between observables [1]. To investigate Efimov phenomenon in three-atomic clusters it is necessary to have a good knowledge of dimer systems [2]. The spectrum of van der Waals rare gas dimers is considered in this presentation.

We calculated spectra and wave functions for pairs of atoms He, Ne, Ar, Kr, Xe and Rn. Calculations were performed for all possible homogeneous and heterogeneous pairs of rare gas atoms. The interatomic van der Waals potentials for the these pairs were determined using the Tang-Toennies [3], Aziz [4] and Lennard-Jones [5] potential models. It is necessary to point out that during purely theoretical *ab initio* computations of potential curves, their authors, as a rule, do not go beyond the presentation of potential values in the form of a table. Such numerical reports are often sufficient, because subsequent application of various parameter-fitting procedures yields fairly simple expressions, but for few-body calculations the analytic expression of potential is needed. The radial wave functions for the ground states of Ne – Rn dimers for the Tang-Toennies potential [3] are presented in the figure (Fig. 1).

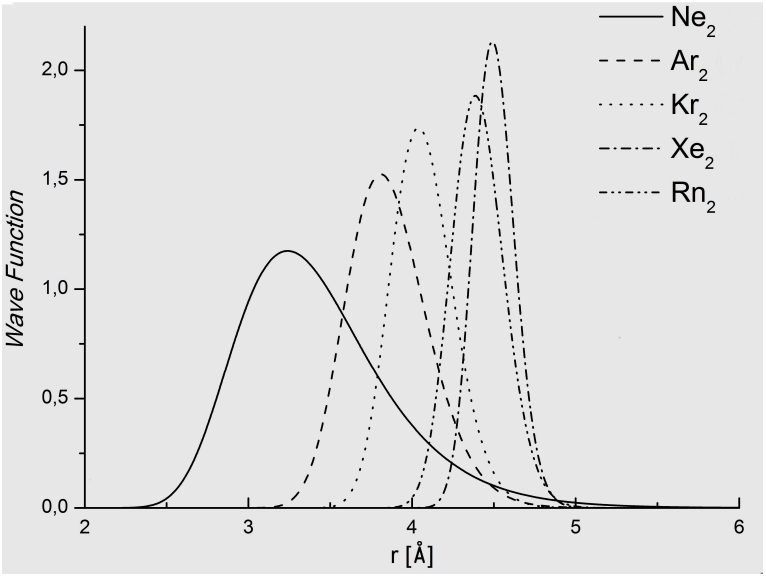

Figure 1: *Radial wave functions of the ground states Ne – Rn dimers for TT potential [3].*

References

[1] H.W. Hammer and L. Platter Ann. Rev. Nucl.Part.Sci. **60**, 207–236 (2010); V.Roudnev and M.Cavagner Phys.Rev.Lett. **108**, 110402 (2012); E.A. Kolganova Few-Body Syst. **4** (2014)
[2] E.A. Kolganova, A.K. Motovilov and W. Sandhas Few-Body Syst. **51**, 249–257 (2011)
[3] K.T. Tang and J.P. Toennies J.Chem.Phys. **118**, 4976-4983 (2003)
[4] R.A. Aziz and M.J. Slaman, J. Chem. Phys. **94**, 8047–8053 (1991); D.A. Barrow, M.J. Slaman and R.A. Aziz J. Chem. Phys. **91**, 6348–6358 (1989); R.A. Aziz J. Chem. Phys. **99**, 4518–4525 (1993)
[5] D.M. Leither, J.D. Doll and M. Whitnell J.Chem.Phys. **94**, 6644 - 6659 (1991)