Michał Hapka

Lista publikacji

z dnia 31 października 2014

Publikacje w czasopismach

1. Hapka M., Rajchel Ł, Modrzejewski M., Chałasiński G., Szczęśniak M. M., 2014, **Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory**, J. Chem. Phys. 141, 134120.

2. Koppen J. V., Hapka M., Modrzejewski M., Szczęśniak M. M., Chałasiński G., 2014, **Density functional theory approach to gold-ligand interactions: Separating true effects from artifacts**, J. Chem. Phys. 140, 244313.

3. Jankunas J., Bertsche B., Jachymski K., Hapka M., Osterwalder A., 2014, **Dynamics of gas phase Ne* + NH_3 and Ne* + ND_3 Penning ionisation at low temperatures**, J. Chem. Phys. 140 , 244302.

4. Hapka M., Kłos J., Korona T., Chałasiński G., 2013, **Theoretical Studies of Potential Energy Surface and Bound States of the Strongly Bound He(^{1}S)-BeO($^1\Sigma^+$) Complex**, J. Phys. Chem. A 177 , 6657.

5. Hapka M., Chałasiński G., Kłos J., Żuchowski P. S., 2013, **First-principles interaction potentials for metastable He(^{3}S) and Ne(^{3}P) with closed-shell molecules: Application to Penning-ionizing systems**, J. Chem. Phys. 139, 014307.

6. Hapka M., Żuchowski P. S., Szczęśniak M. M, Chałasiński, 2012, **Symmetry-adapted perturbation theory based on unrestricted Kohn-Sham orbitals for high-spin open-shell van der Waals complexes**, J. Chem. Phys. 137, 164104.

7. Koppen J. V., Hapka M., Szczęśniak M. M., Chałasiński G., 2012, **Optical absorption spectra of gold clusters Au_n (n = 4, 6, 8, 12, 20) from long-range corrected functionals with optimal tuning**, J. Chem. Phys. 137 , 114302.

8. Sayfutyarova E. R., Buchachenko A. A., Hapka M., Szczęśniak M. M., Chałasiński G., 2012, **Interactions of ThO (X) with He, Ne and Ar from the ab initio coupled cluster and symmetry adapted perturbation theory calculations**, Chem. Phys. 339 , 50.

9. Rajchel Ł, Żuchowski P. S., Hapka M., Modrzejewski M., Szczęśniak M. M., Chałasiński G., 2010, **A density functional theory approach to noncovalent interactions via interacting monomer densities**, Phys. Chem. Chem. Phys. 12 , 14686.

10. Kiersztan A., Barańska A., Hapka M., Lebiedzinska M., Winiarska K., Dudziak M., Bryła J., 2009, **Differential action of methylselenocysteine in control and alloxan-diabetic rabbits**, Chem Biol Interact. 177 , 161 (2009)