Квантово-химические расчеты димеров оганесона и его гомологов

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Motivation

Determining the limits of applicability of the Mendeleev's periodic law:

- Investigation of properties in comparison with homologues in the noble gases group.
- Investigation of the relativistic effects contribution to molecular properties.
- 2-particle interaction potentials for molecular dynamics methods $\rightarrow$ thermodynamic properties.

Methods

Hamiltonian:

Relativistic → Non-Relativistic with pseudopotential

Mosyagin N.S., Zaitsevskii A.V., Titov A.V. (2020)
GRECP - Generalized Relativistic Effective Core Potential:
For Og atom:
– replaces 92 electrons with pseudopotential leaving us overall with a problem for the $6s^2 6p^6 6d^{10} 7s^2 7p^6$ configuration,
– allows to take into account relativistic effects and Breit interaction.

Electronic correlation:

Coupled-cluster method – CCSD(T)
Programs - DIRAC, CFOUR

Basis set

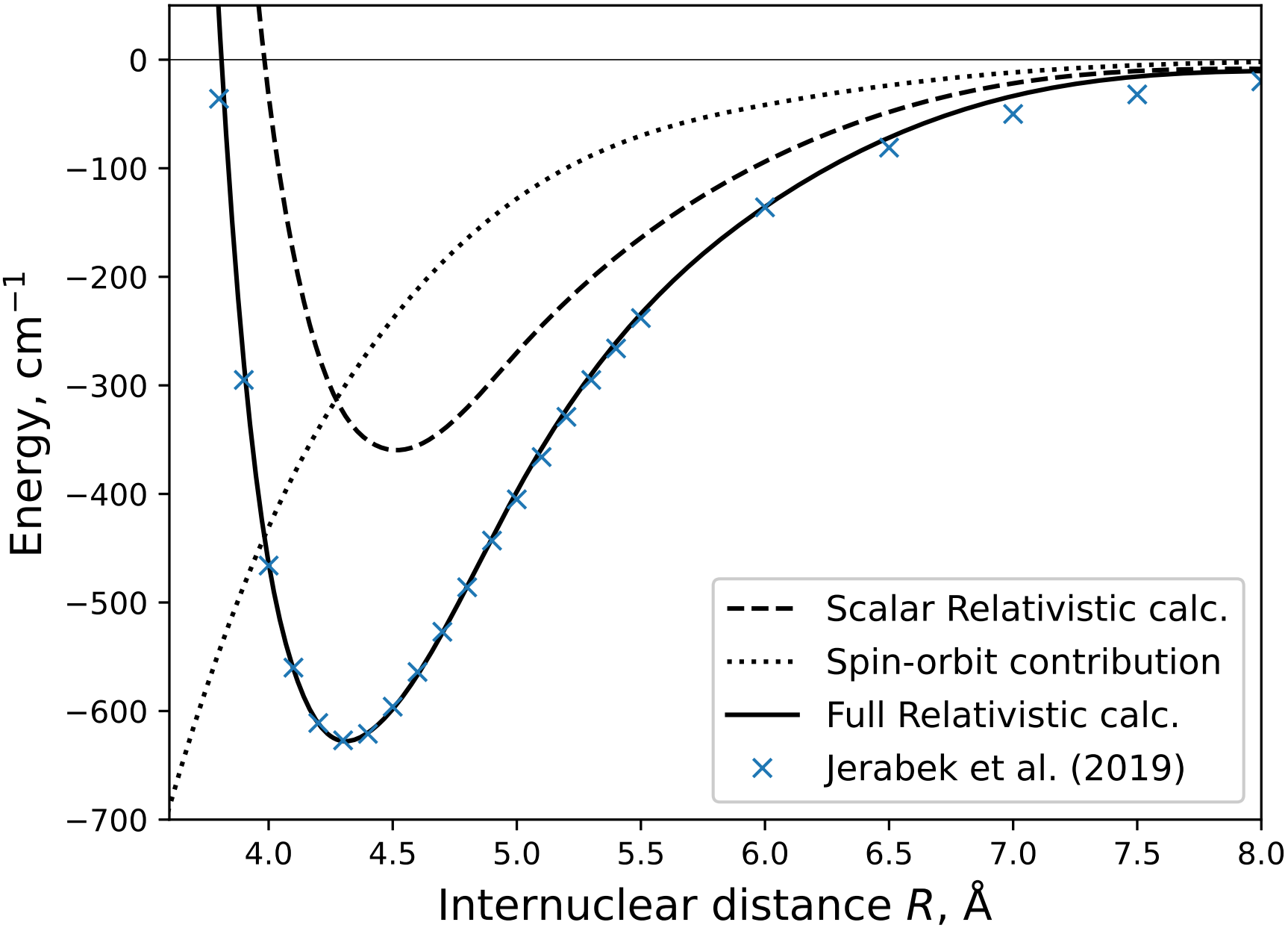
Gaussian Type Orbitals:

$$R_l^\alpha = N_l^\alpha r^l e^{-\alpha r^2}, \qquad l = 0(s), 1(p), 2(d)...$$

Kaygorodov M. Y. et al. //Physical Review A. – (2021):
$19s17p14d12f4g3h3i$ – basis set optimized on FSCC-SD calculations of electron affinity of Og.

Other approaches:
Jerabek P. et al. (2019): Construction of several smaller basis sets and extrapolation to complete basis set.
Shee A., Knecht S., Saue T. (2015); de Macedo L. G. M. et al. (2023) – Standard basis sets.

Og_2 potential energy curve

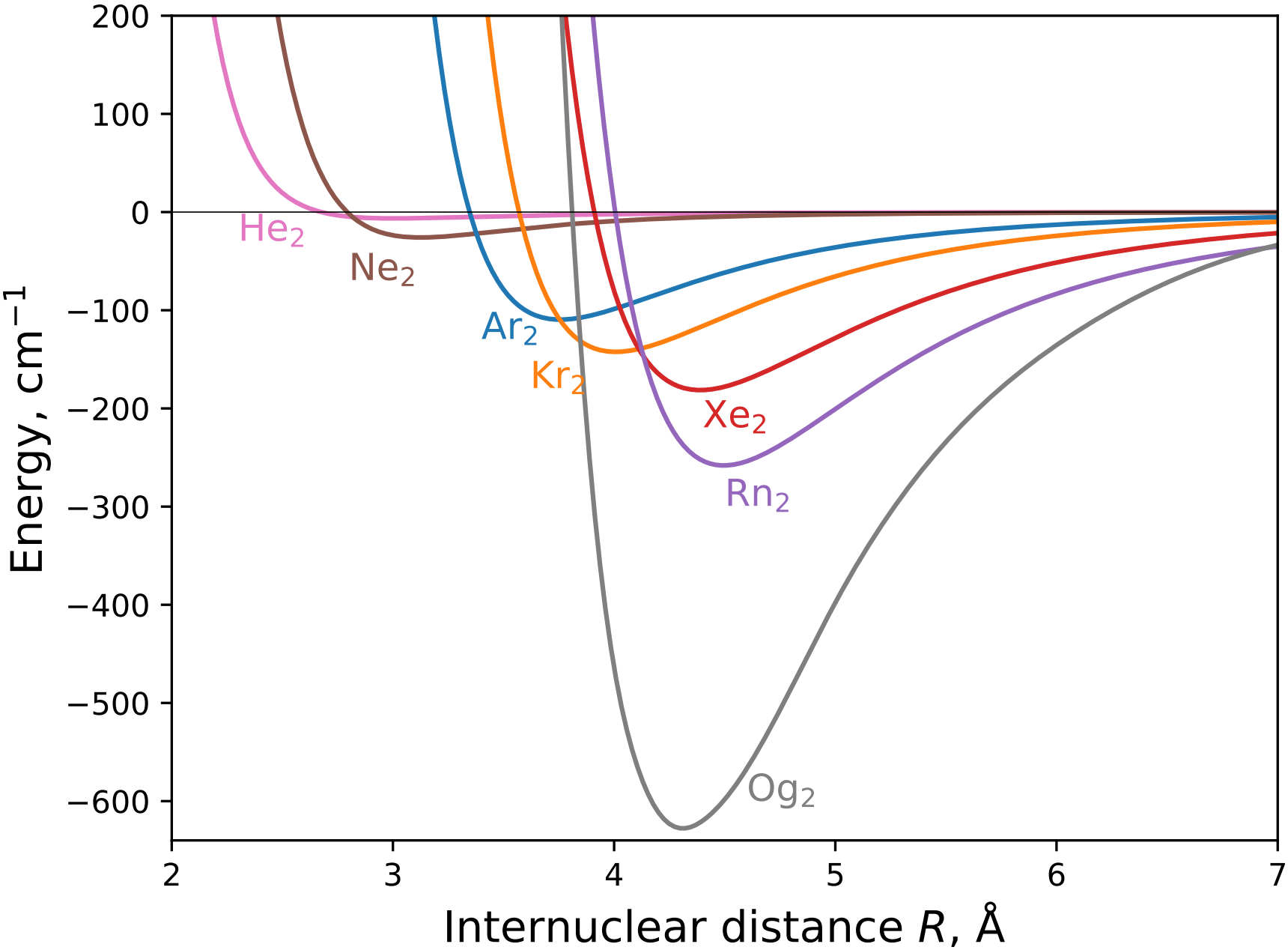


Og_2 molecular properties

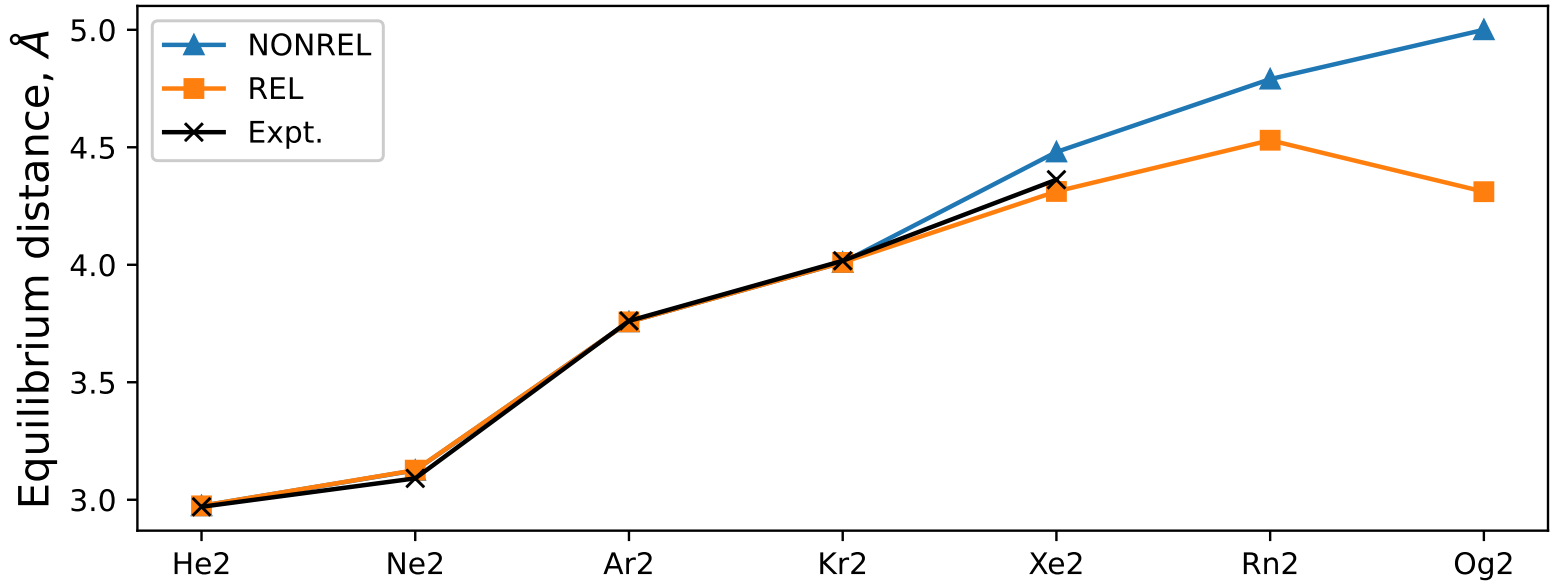
	D_e, cm^{-1}	R_e, Å
CCSD(T) Scalar-Relativistic	360	4.515
CCSD(T) Full Relativistic	628	4.311
CCSDT(Q) Scalar-Relativistic[1]	366.17	4.4923
CCSDT(Q) Full Relativistic[1]	626.69	4.3137
CCSD(T)[2]	624.24	4.329
MP2-srLDA[3]	843.50	4.25

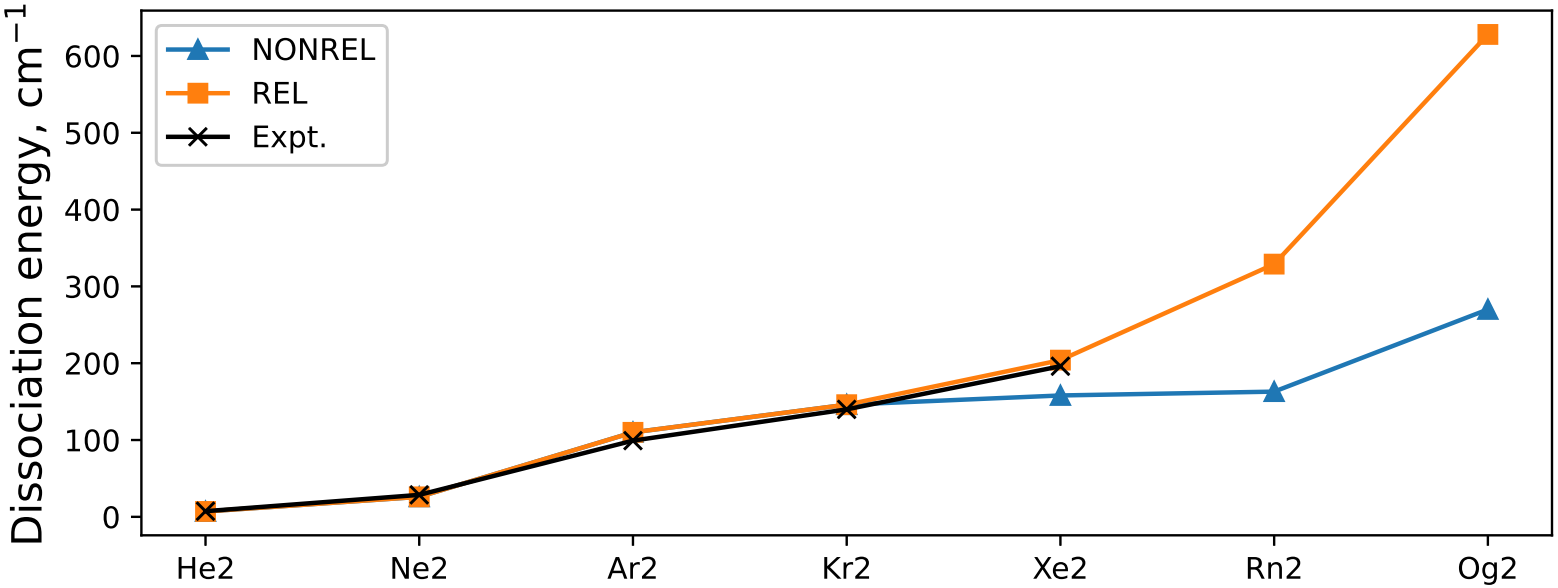
[1] Jerabek P. et al. (2019)
[2] Shee A., Knecht S., Saue T. (2015)
[3] de Macedo L. G. M. et al. (2023)

Noble gas dimers: potential energies



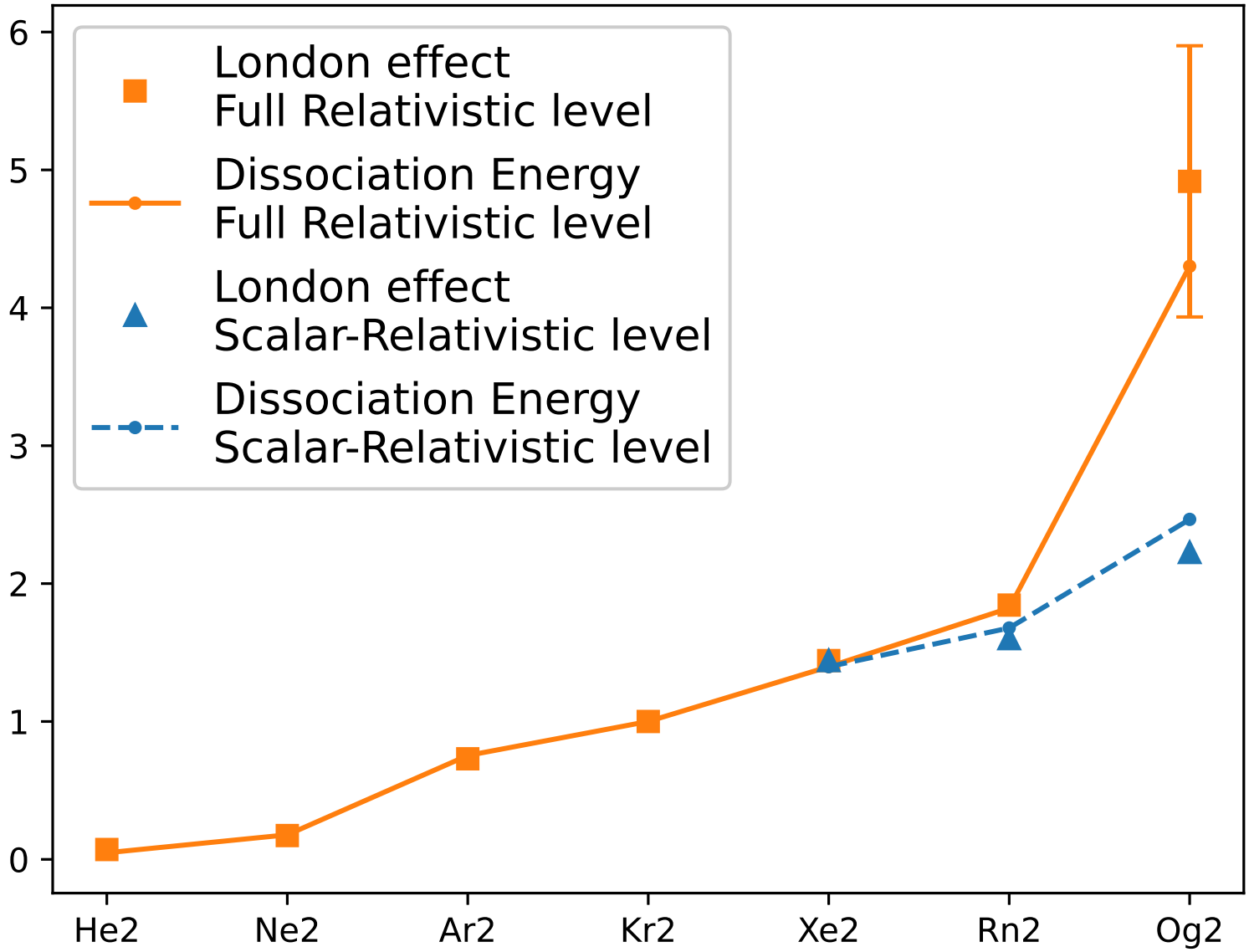
Noble gas dimers: molecular properties





London effect $\frac{I\alpha^2}{R^6}$

I – ionization potential, α – polarizability.



Thank you for your attention