Supporting Information

Molecular Structures, Energetics and Electronic Properties of Neutral and Charged Hg_n Clusters (n= 2–8)

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Table S1. In order to investigate the effects of the basis sets and exchange-correlation functionals on the mercury dimer, we use various types of functionals (LDA, GGA, and hybrid functional) and basis sets for the Hg_2 test calculation. Bond length r_e (in Å), binding energies D_e (in eV) and vibrational frequencies ω_e (in cm^{-1}) calculation results for the Hg_2 with various DFT functionals and MP2 method are summarized

	r_e (Å)				ω_e (cm^{-1})				D_e (eV)			
	TZ	QZ	5Z	pwCVTZ	TZ	QZ	5Z	pwCVTZ	TZ	QZ	5Z	pwCVTZ
LDA	3.017	3.010	3.01 4	3.016	53.3	54.7	54.0	53.5	0.236	0.237	0.234	0.231
PW91	3.525	3.518	3.517	3.522	28.2	28.3	28.2	28.2	0.047	0.047	0.047	0.046
PBE	3.562	3.554	3.552	3.559	26.2	26.6	26.6	26.3	0.038	0.038	0.037	0.036
mPWPW91	3.620	3.607	3.608	3.621	18.1	20.3	19.8	17.7	0.012	0.013	0.011	0.001
B3LYP	4.339	4.329	4.334	4.347	11.3	11.4	11.4	11.1	-0.002	-0.002	-0.003	-0.003
PBE0	3.626	3.614	3.614	3.622	18.9	20.2	20.1	19.2	0.029	0.029	0.028	0.027
mPW1PW91	3.812	3.787	3.805	3.820	12.4	9.8	11.3	12.7	0.011	0.011	0.009	0.009
M06-L	3.504				30.8				0.059			
M06	3.502				31.7				0.066			
MP2	3.320	3.275	-	3.351	33.0	33.8	-	31.6	0.146	0.146	-	0.125
Exp.	3.63 ± 0.04				19.6 ± 0.3				0.043 ± 0.003			

Hg basis set
K. A. Peterson and C. Puzzarini, *Theor. Chem. Acc.*, **2005**, *114*, 283.

Exp. value of r_e from van Zee RD, Blankkespoor SC and Zwier TS , *J. Chem. Phys*., **1998**, 88, 4650., ω_e from Koperski J, Atkinson JB and Krause L, *Can. J. Phys.,* **1994**, 72, 1070., D_e fromZehnacker A, Duval M.C, Jouvet C, Lardeux-Dedonder C, Solgadi D., Soep B, Benoist d'Azy, *O. J. Chem. Phys.*, **1987**, 86, 6565.

TZ: aug-cc-pVTZ-PP [6s6p5d3f2g]
QZ: aug-cc-pVQZ-PP [7s7p6d4f3g2h]
5Z: aug-cc-pV5Z-PP [8s8p7d5f4g3h2i]
pwCVTZ: aug-cc-pwCVTZ-PP [8s8p7d4f3g]