Supporting information for: Quantum chemical study of hydrogen adsorption on carbon-supported palladium clusters

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Comparison of three different functionals for the hydrogen adsorption energy on free Pd_6

functional	ΔE_{ads} in kJ/mol
TPSS	-49.2
PBE	-63.4
BP86	-61.0

Comparison of two different basis sets for the hydrogen adsorption energy on free Pd_6

basis set	ΔE_{ads} in kJ/mol
def2-SVP	-49.2
def2-TZVP	-38.2

Comparison of three different functionals for the incremental adsorption energies for an increasing number of H_2 molecules on free Pd_6 in kJ/mol

number of H_2	TPSS	PBE	BP86
1	-49.2	-70.5	-60.4
2	-43.8	-65.5	-54.8
3	-43.7	-68.2	-56.5
4	-37.8	-59.2	-48.2
5	-33.7	-54.8	-43.4
6	-24.2	-41.6	-29.8
7	-64.8	-112.7	-103.3

Comparison of two different basis sets for the incremental adsorption energies for an increasing number of H_2 molecules on free Pd_6 in kJ/mol

number of H_2	def2-SVP	def2-TZVP
1	-49.2	-59.6
2	-43.8	-41.4
3	-43.7	-49.8
4	-37.8	-54.6
5	-33.7	-39.8
6	-24.2	-31.8
7	-64.8	-64.0

Comparison of two different functionals for the dispersion contribution to the metal-support interactions in the Pd_6 system

functional	total binding energy in kJ/mol	dispersion contribution in kJ/mol
TPSS	195.7	95.0
PBE	172.9	70.3

Comparison of two different functionals for the dispersion contribution to the metal-support interactions in the Pd_{21} system

functional	total binding energy in kJ/mol	dispersion contribution in kJ/mol
TPSS	549.7	301.5
PBE	451.0	220.0