**Supporting Information**

# On the Role of Long Range Interactions for the Structure and Energetics of Olympicene Radical Adsorbed on Au(111) and Pt(111) Surfaces

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**Table S1.** Optimized bulk lattice constants (in Å) for Au and Pt obtained using PBE, optB86b-vdW, optB88-vdW, optPBE-vdW, revPBE-vdW, and rPW86-vdW2 functionals were summarized in an earlier publication.[1] The experimental lattice constants with the zero-point energy corrections (ZPEC) are taken from the reference[2] to provide comparison.

| Method | Au | Pt |
|---|---|---|
| **PBE** | 4.170 | 3.980 |
| **optB86b-vdW** | 4.140 | 3.960 |
| **optB88-vdW** | 4.178 | 3.988 |
| **optPBE-vdW** | 4.197 | 3.999 |
| **revPBE-vdW** | 4.261 | 4.040 |
| **rPW86-vdW2** | 4.352 | 4.117 |
| **Experiment** | 4.061[2] | 3.913[2] |

1. Yildirim, H.; Greber, T.; Kara, A., Trends in Adsorption Characteristics of Benzene on Transition Metal Surfaces: Role of Surface Chemistry and Van Der Waals Interactions. *J. Phys. Chem. C* **2013**, *117*, 20572-20583.

2. Hao, P.; Fang, Y.; Sun, J.; Csonka, G. I.; Philipsen, P. H.; Perdew, J. P., Lattice Constants from Semilocal Density Functionals with Zero-Point Phonon Correction. *Phys. Rev. B* **2012**, *85*, 014111.