# Hybrid Organic/TMD Heterostructures for Photovoltaic Applications

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Two-dimensional transition metal dichalcogenides (TMDs) are considered encouraging materials for photovoltaic applications [1], with differing electronic and optical properties from their bulk counterparts. Pentacene is an organic compound with high carrier mobility [2], and complimentary electronic properties to TMDs. Pentacene/MoS2 hybrid heterostructures have been investigated previously with promising results [3]. Here are investigated systems of adsorbed pentacene on monolayers of Group-VI transition metal dichalcogenides; MoS2, MoSe2, WS2 and WSe2, for photovoltaic applications. Using ab initio methods with HSE and van der Waals corrections of underlying density functional theory (DFT), optimized atomic positions were calculated and energetically favourable adsorption sites of pentacene were determined. The most favorable sites were further investigated with analysis of band gap alignment between the hybrid substrate and adsorbate. Density of States, band structure and charge density analysis were then performed.

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## References

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[2] S. F. Nelson, Y.-Y. Lin, D. J. Gundlach, and T. N. Jackson. Applied Physics Letters, vol. 72, no. 15, 1998. pp. 1854–1856.
[3] S. Bettis Homan, V. K. Sangwan, I. Balla, H. Bergeron, E. A. Weiss, and M. C. Hersam. Nano Letters, vol. 17, no. 1, 2017. pp. 164–169.

## Figures

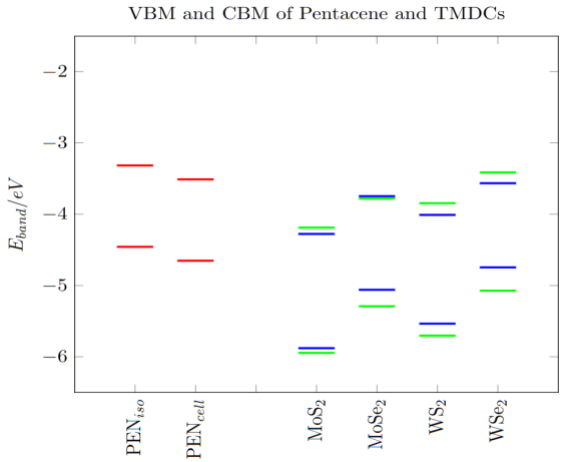


**Figure 1:** Frontier orbitals (DFT) of isolated pentacene, pentacene within a supercell defined by TMDs, and the investigated TMDs with (blue) and without (green) spin-orbit coupling.