

# Recipes for Few-layer Black Phosphorus Functionalization

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## Abstract

Few-layer black phosphorus or phosphorene is 2D material obtained by the exfoliation of black phosphorus. [1] Beside of interesting properties of the material, one of its major drawback is the high sensitivity toward atmospheric oxygen and moisture. Covalent and non-covalent functionalization is one common protection strategy. During the last few years, we have developed *in silico* recipes for the development of functionalized surfaces and predict electronic properties for future applications. [2] From the isolobal analogy, we recognized the similarity of phosphorene with graphane, the all hydrogenated version of graphene. Moreover, the presence of a lone pairs at the top of the valence suggested to look at phosphorene as an extended phosphine with lone pairs waiting for reacting with the right metal fragments or Lewis acid. The donor strength of the phosphorene lone pairs was compared with other molecular P donors from a phosphine to white phosphorus and phosphorene is one of the weakest. Never the less, we predicted several candidates for the functionalization. Starting from our work, some interesting modification of the phosphorene material have been recently reported by our group [3] and by other authors [4].

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