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Functionalized 2D atomic sheets with new properties QIANG SUN, JIAN ZHOU, Peking University, QIAN WANG, PURU JENA, Virginia Commonwealth University — Due to the unique atomic structure and novel physical and chemical properties, graphene has sparked tremendous theoretical and experimental efforts to explore other 2D atomic sheets like B-N, Al-N, and Zn-O, where the two components offer much more complexities and flexibilities in surface modifications. Using First principles calculations based on density functional theory, we have systematically studied the semi- and fully-decorated 2D sheets with H and F and Cl. We have found that the electronic structures and magnetic properties can be effectively tuned, and the system can be a direct or an indirect semiconductor or even a half-metal, and the system can be made ferromagnetic, antiferromagnetic, or magnetically degenerate depending upon how the surface is functionalized. Discussions are made for the possible device applications.

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