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Macrocycles inserted in graphene: from coordination chemistry on graphene to graphitic carbon oxide.[1] WEI LIU, Beijing Computational Science Research Center, JINGYAO LIU, Institute of Theoretical Chemistry, Jilin University, MAOSHENG MIAO, California State University Northridge — Tuning the electronic structure and the chemical properties of graphene by binding with metals has become a focus in the area of two dimension materials. Despite many interesting results and promising potentials, the approach suffers from weak binding and the high reactivity of the metal atoms. On the other hand, many macrocyclic molecules such as crown ether show strong and selective binding with metal atoms. The alliance of the two substances will largely benefit the two parallel fields: it will provide a scaffold for coordination chemistry as well as a controllable method for tuning the electronic structure of graphene through strong binding with metals. Here, using crown ether as an example, we demonstrate by first principles calculations that the embedment of macrocyclic molecules into graphene honeycomb lattice can be very thermochemically favored. The embedment of crown ether on graphene can form a family of new two-dimensional materials that possess varying band gaps and band edges. The one with highest O composition (C_2O), with similar structure features as graphilic C_3N_4, shows strong potentials for photolysis and as true two-dimensional superconductor while binding with alkali metals.

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