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Design of Ordered Graphene Oxides by First-Principles based Cluster Expansion Approach BING HUANG, NREL, HONGJUN XIANG, NREL-Fudan, SUHUAI WEI, NREL — The inhomogeneous phase, which usually exists in graphene oxides (GOs), is a long-standing problem that has severely restricted the use of GOs in various applications. By using first-principles based cluster expansion, we find that the existence of phase separation in conventional GOs is due to the extremely strong attractive interactions of oxygen atoms at different graphene sides. Our Monte Carlo simulations show that this kind of phase separation is not avoidable under the current experimental growth temperature. In this Letter, the idea of oxidizing graphene on single-side is proposed to eliminate the strong double-side oxygen attractions, and our calculations show that well-ordered GOs could be obtained at low oxygen concentrations. These ordered GOs behave as quasi-one-dimensional narrow-gap semiconductors with quite small electron effective masses, which can be useful in high-speed electronics. Our concept could be widely applied to overcome the inhomogeneous phases in various chemically functionalized two-dimensional systems.

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