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Electronic and transport properties in graphene oxide frameworks PAN ZHU, VINCENT MEUNIER, Rensselaer Polytechnic Institute — We report a detailed theoretical study of the electronic and transport properties of a series of graphene oxide frameworks (GOFs) using first-principles calculations based on density functional theory. The pillar molecular structure of GOFs determine that with various linear boronic acid pillars and different pillar concentrations, GOF structures can be fine tuned and exhibit various electronic properties. Based on ideal GOF structures, we predict that GOFs' electronic properties, such as band gap, can be modified controllobly by an appropriate choice of pillaring units and pillar concentration. The quantum transport properties of several systems with various linear boronic acid pillars are also evaluated. The variation of conductance arising from different pillar composition is shown to be potentially useful for practical applications.

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