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Theoretical Study of Carborane:Pyridine and Carborane:Pyrimidine Aggregates and Polymers. YI GAO, ZHONG-KANG HAN, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, NAN SHAO, WAI-NING MEI, University of Nebraka-Omaha — The carboranes are cross-linked by the pyridines and pyrimidines to form aggregates and polymers. Their geometries and electronic structures are studied by the first-principle calculations. Our results show different connections influence the orientations of the aromatic rings of pyridines and pyrimidines, which would highly affect the electronic structures of carborane:pyridine and carborane:pyrimidine aggregates and polymers. This study might be helpful for the future design of new class of semiconducting boron carbides.

Yi Gao
Shanghai Institute of Applied Physics, Chinese Academy of Sciences

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