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标题: Graphene-Based Vibronic Devices

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摘要: Molecular dynamic simulations are used to model the vibrational bending modes of graphene ribbons of several sizes to calculate frequencies of the ribbons and determine the relationship between the size of the ribbon and their corresponding resonance frequencies. These ribbons can be utilized to fabricate several types of vibronic devices such as NEMS, sensors, terahertz generators, and devices for encoding, transferring, and processing information. The interaction of a graphene vibronic device with water and isopropyl alcohol molecules demonstrates that this device can be used as a very sensitive vibronic molecular sensor that is able to distinguish the chemical nature of the sensed molecule. The electrical properties of the graphene vibronic devices are also calculated for two cases, armchair and zigzag border. The zigzag border demonstrated in this work has the potential to generate THz electrical signals.

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