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Supporting Materials for Thermal and electrical transport properties of two-dimensional Dirac graphenylene: a first-principles study

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1、Band structures calculated by HSE06 functional for graphenylene

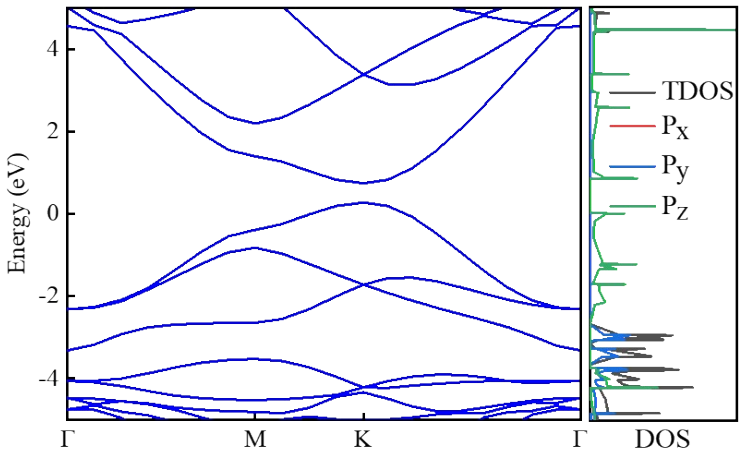

Figure S1. Band structures calculated by HSE06 functional for graphenylene.

2. The radial distribution function of graphenylene

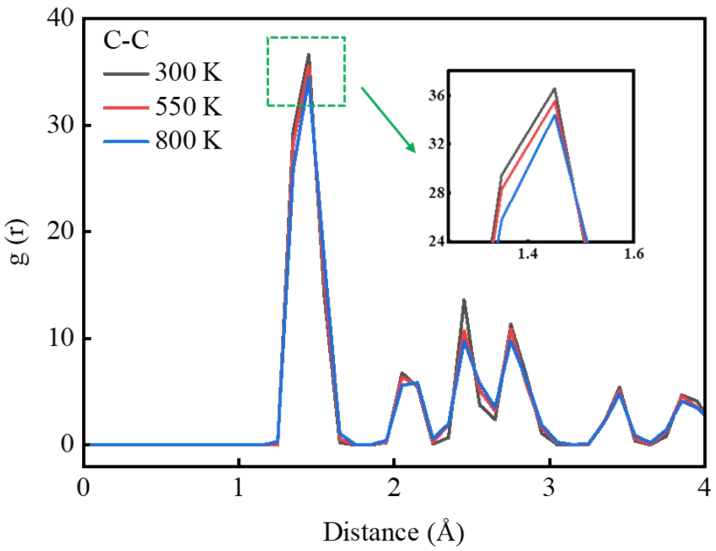

Figure S2. The radial distribution function of graphenylene.

3. Lattice parameters and atomic fractional positions for graphenylene

System	Lattice parameters	Fractional coordinates
graphenylene	a = 6.769 Å, b = 11.724 Å, c = 20.0 Å, θ = 90°	C1 (0.609, 0.063, 0.499), C2 (0.109, 0.563, 0.499), C3 (0.600, 0.272, 0.499), C4 (0.100, 0.772, 0.499), C5 (0.290, 0.163, 0.499), C6 (0.790, 0.663, 0.499), C7 (0.390, 0.936, 0.499), C8 (0.890, 0.436, 0.499), C9 (0.399, 0.727, 0.499), C10 (0.899, 0.227, 0.499), C11 (0.709, 0.836, 0.499), C12 (0.209, 0.336, 0.499), C13 (0.609, 0.936, 0.499), C14 (0.109, 0.436, 0.499), C15 (0.600, 0.727, 0.499), C16 (0.100, 0.227, 0.499), C17 (0.290, 0.836, 0.499), C18 (0.790, 0.336, 0.499), C19 (0.390, 0.063, 0.499), C20 (0.890, 0.563, 0.499), C21 (0.399, 0.272, 0.499), C22 (0.899, 0.772, 0.499), C23 (0.709, 0.163, 0.499), C24 (0.209, 0.663, 0.499)

Table S1. Lattice parameters and atomic fractional positions for graphenylene.