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Anisotropic mechanical properties of graphene: a molecular dynamics study MING YU, University of Louisville, ANNA ZENG, KEVIN ZENG, Mission San Jose High School — The anisotropic mechanical properties of monolayer graphene with different shapes have been studied using an efficient quantum mechanics molecular dynamics scheme based on a semi-empirical Hamiltonian (refereed as SCED-LCAO) [PRB 74, 15540; PHYSE 42, 1]. We have found the anisotropic nature of the membrane stress. The stresses along the armchair direction are slightly stronger than that along the zigzag direction, showing strong direction selectivity. The graphene with the rectangular shape could sustain strong load (*i.e.*, 20%) in both armchair and zigzag directions. The graphene with the rhombus shape show large difference in the strain direction: it will quickly crack after 18 % of strain in armchair the direction, but slowly destroyed after 20% in the zigzag direction. The obtained 2D Young's modulus at infinitesimal strain and the third-order (effective nonlinear) elastic modulus are in good consistent with the experimental observation.

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