Supporting Information

Critical Role of Surface Defects in the Controllable Deposition of Li_2S on Graphene: From Molecule to Crystallite

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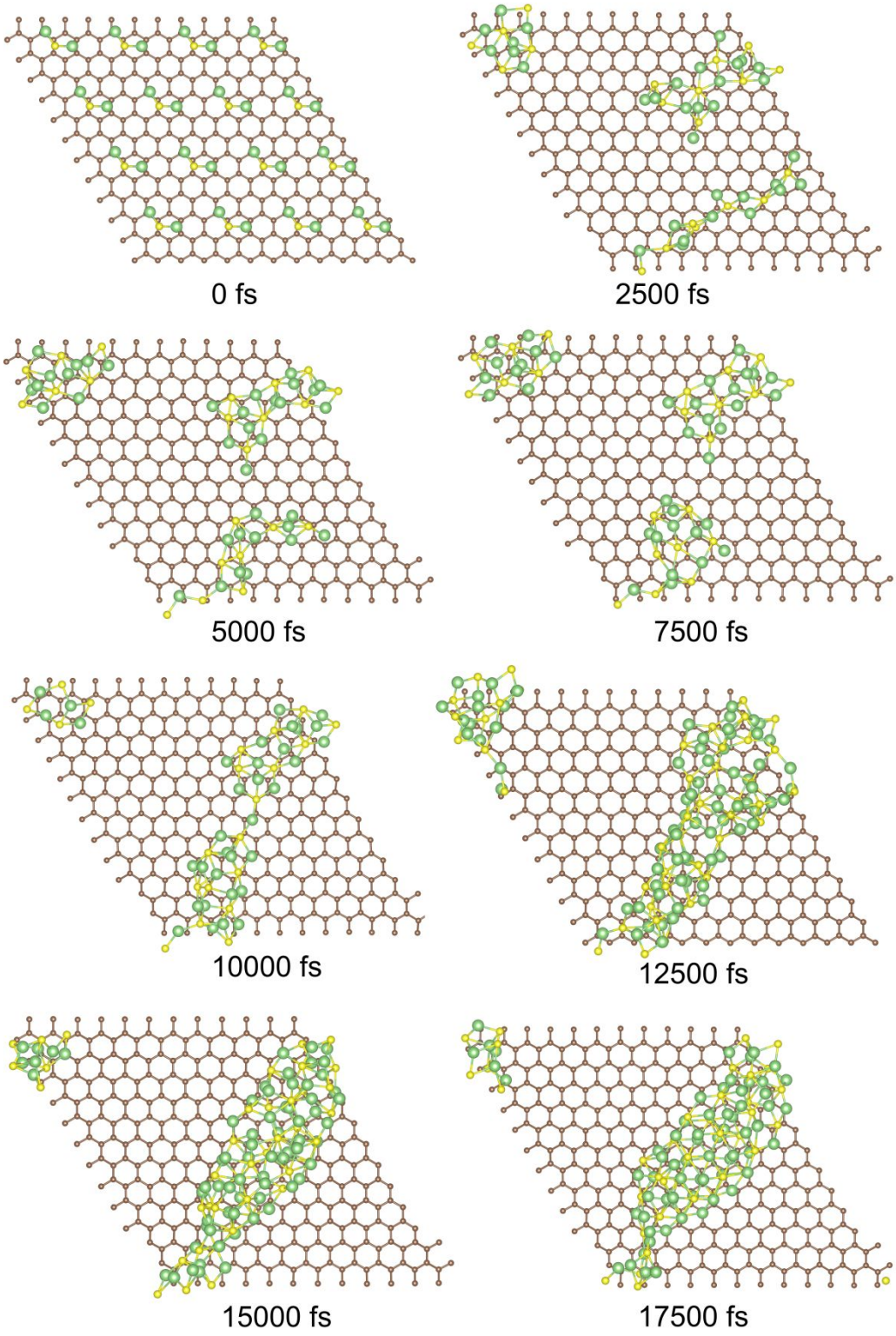

Figure S1. Snapshots of AIMD simulation of Li_2S clusters on pristine graphene at 0, 2500, 5000, 7500, 10000, 12500, 15000, and 17500 fs. The number of Li_2S molecule is doubled after 10000 fs.

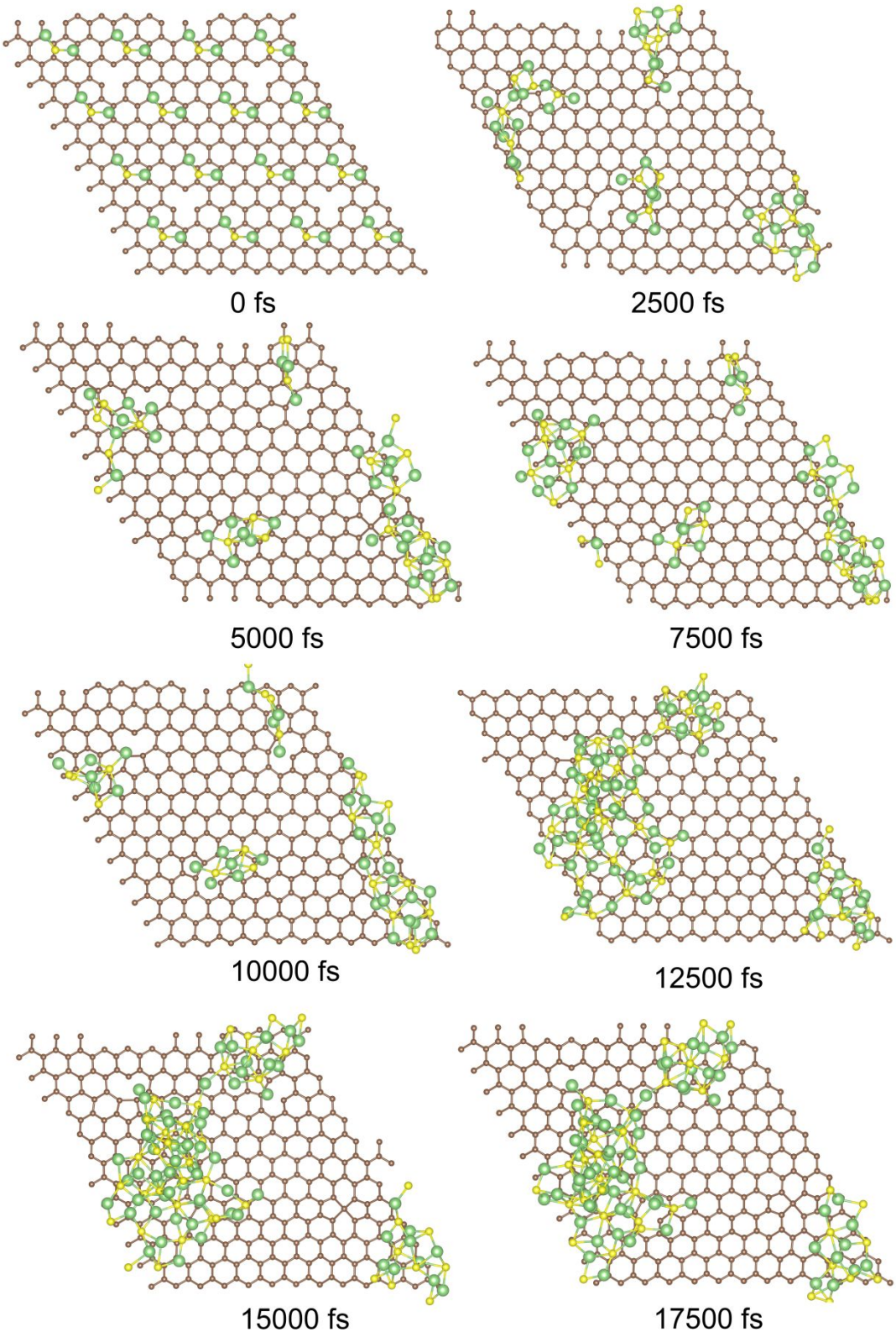

Figure S2. Snapshots of AIMD simulation of Li_2S clusters on SV defected graphene at 0, 2500, 5000, 7500, 10000, 12500, 15000, and 17500 fs. The number of Li_2S molecule is doubled after 10000 fs.

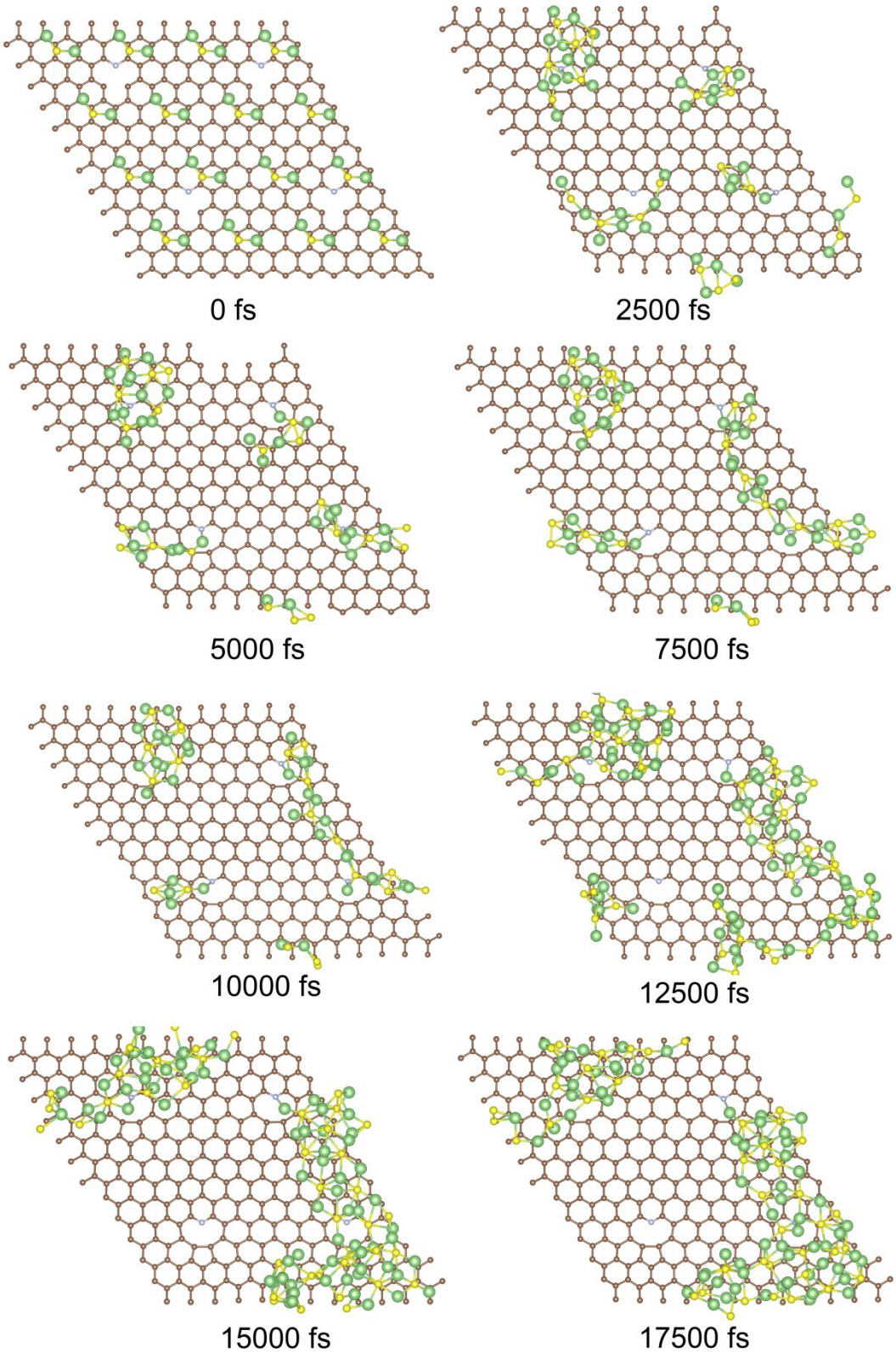

Figure S3. Snapshots of AIMD simulation of Li_2S clusters on PDN-doped graphene at 0, 2500, 5000, 7500, 10000, 12500, 15000, and 17500 fs. The number of Li_2S molecule is doubled after 10000 fs.

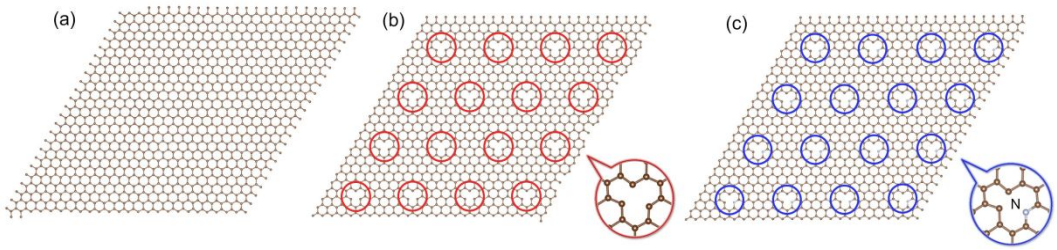

Figure S4. (a) 12×12 pristine graphene substrates, (b) 12×12 SV defected graphene substrates, and (c) 12×12 PDN-doped graphene substrates used for AIMD simulations. The location of SV defects and PDN heteroatoms are circled. The structures are expanded twice in a and b directions periodically for better observation.

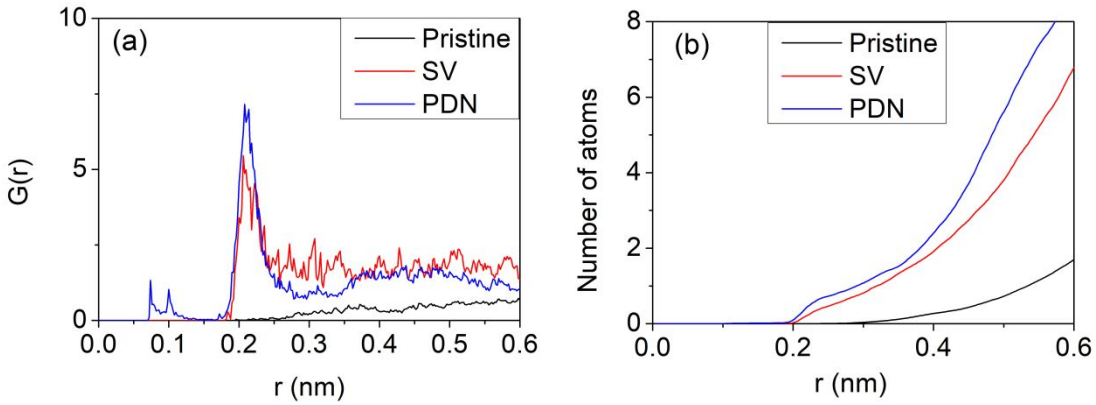

Figure S5 (a) the radial distribution functions (RDF) of Li atoms, (b) the cumulative RDF of Li atoms of Li_2S molecules on pristine, SV defects and PDN doped graphene substrates after 20000 fs of AIMD simulation.

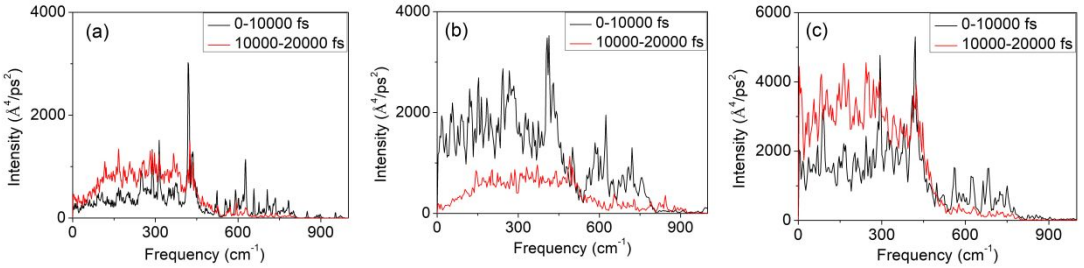

Figure S6 VACF power spectrum of Li_2S clusters deposited on (a) pristine graphene, (b) SV

defected graphene, (c) PD-N doped graphene substrates.

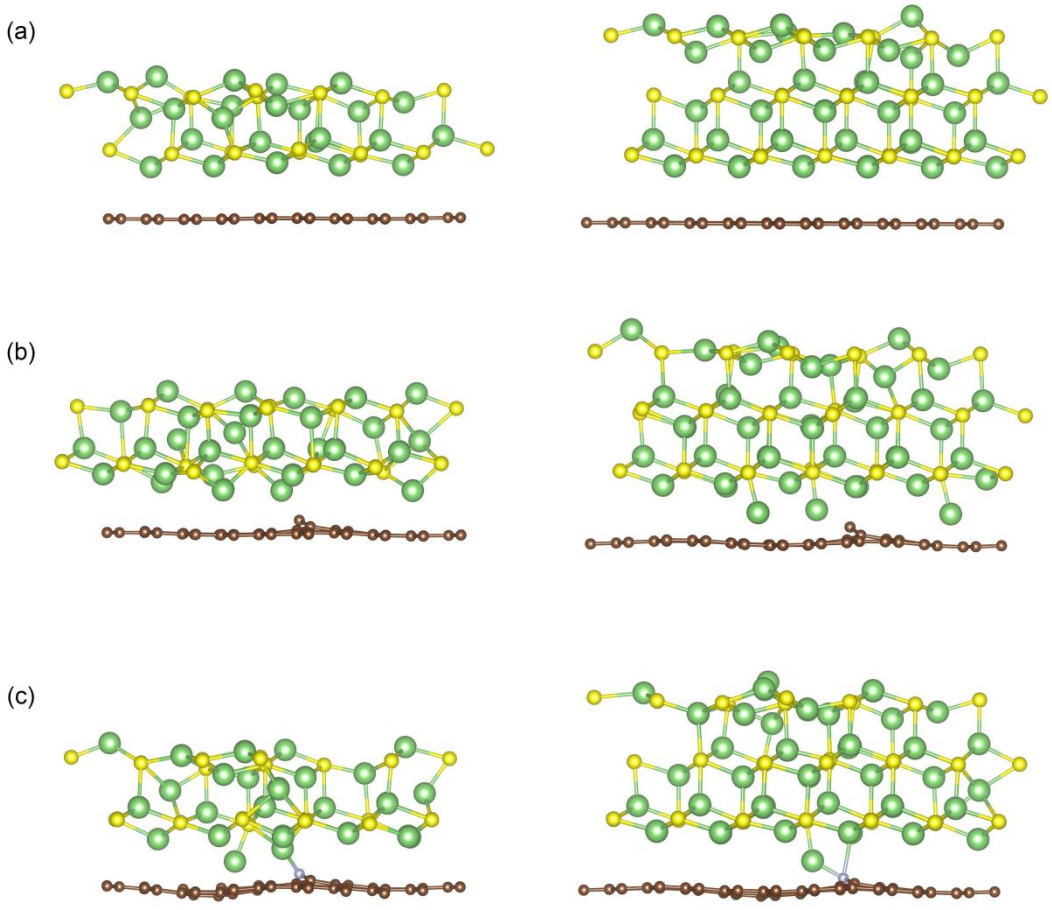

Figure. S7 Optimized structures of the Li_2S-graphene interface containing two and three layers of Li_2S with (a) pristine graphene, (b) SV defected graphene, (c) PDN doped graphene substrates.