Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

Insights into the characterization of interphase thickness in graphene/epoxy nanocomposites: a molecular dynamics simulation

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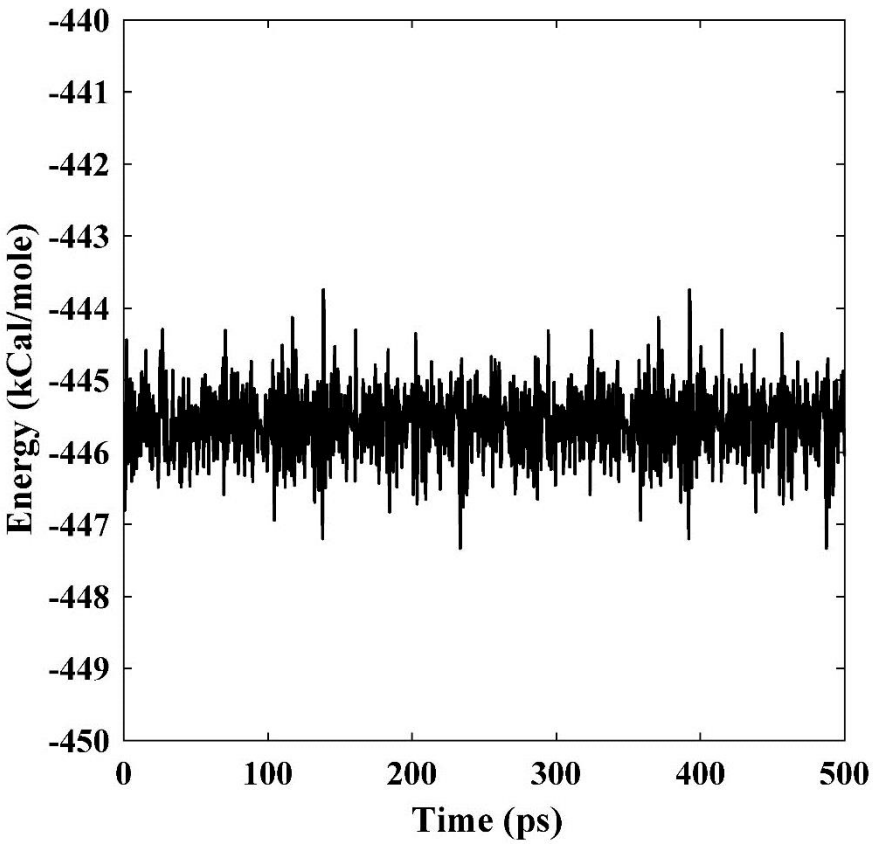

Fig. S1: Evolution of interaction energy during the sampling run for the L5C40 sample

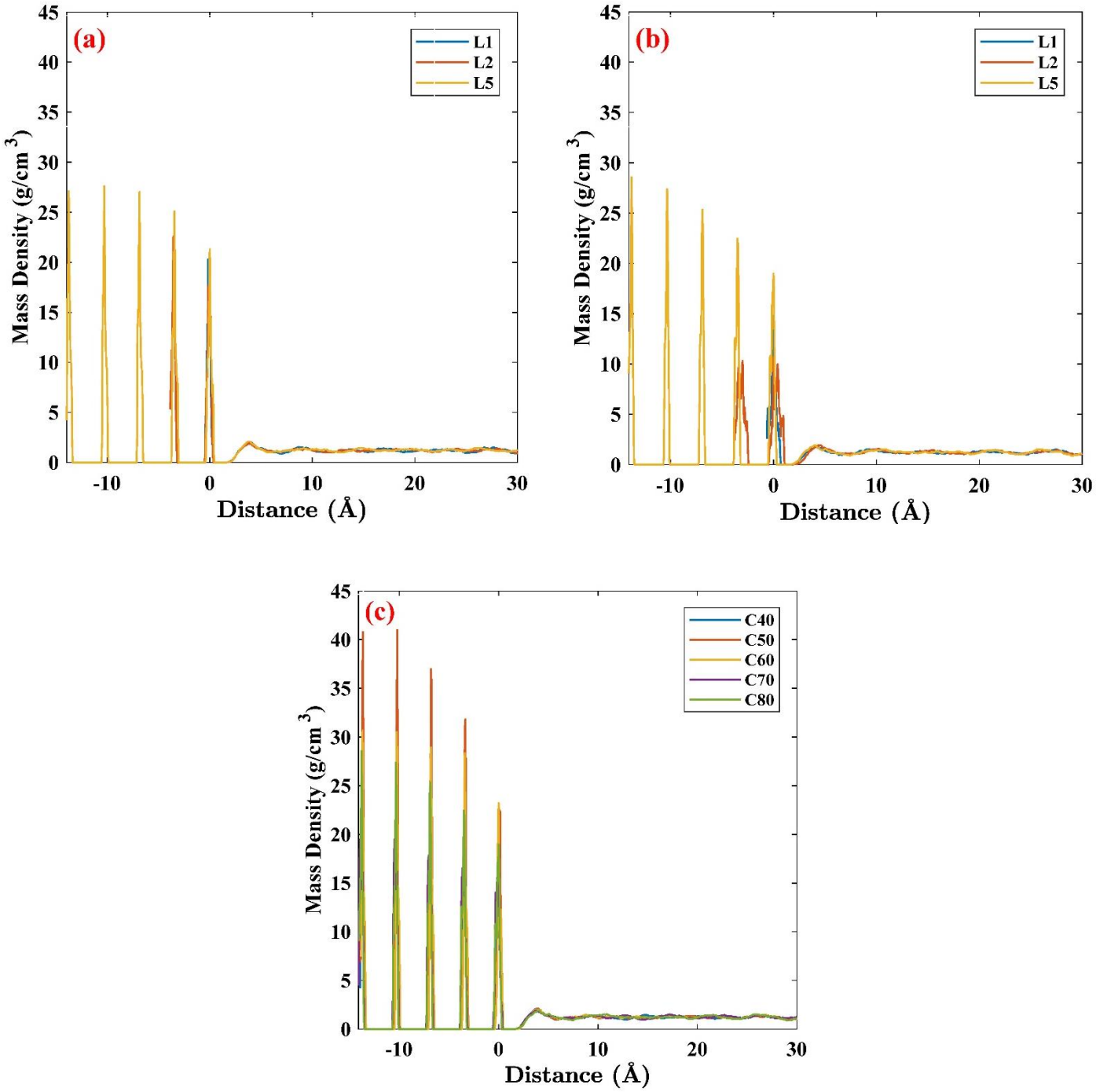

Fig. S2: Mass density profiles along the z-axis of the simulation box for: a) 40% crosslinked and b) 80% crosslinked epoxy in the system with 1, 2, and 5 layers of graphene. c) Mass density profile along the z-axis for the five-layer graphene model with 40%, 50%, 60%, 70%, and 80% crosslinked epoxy.

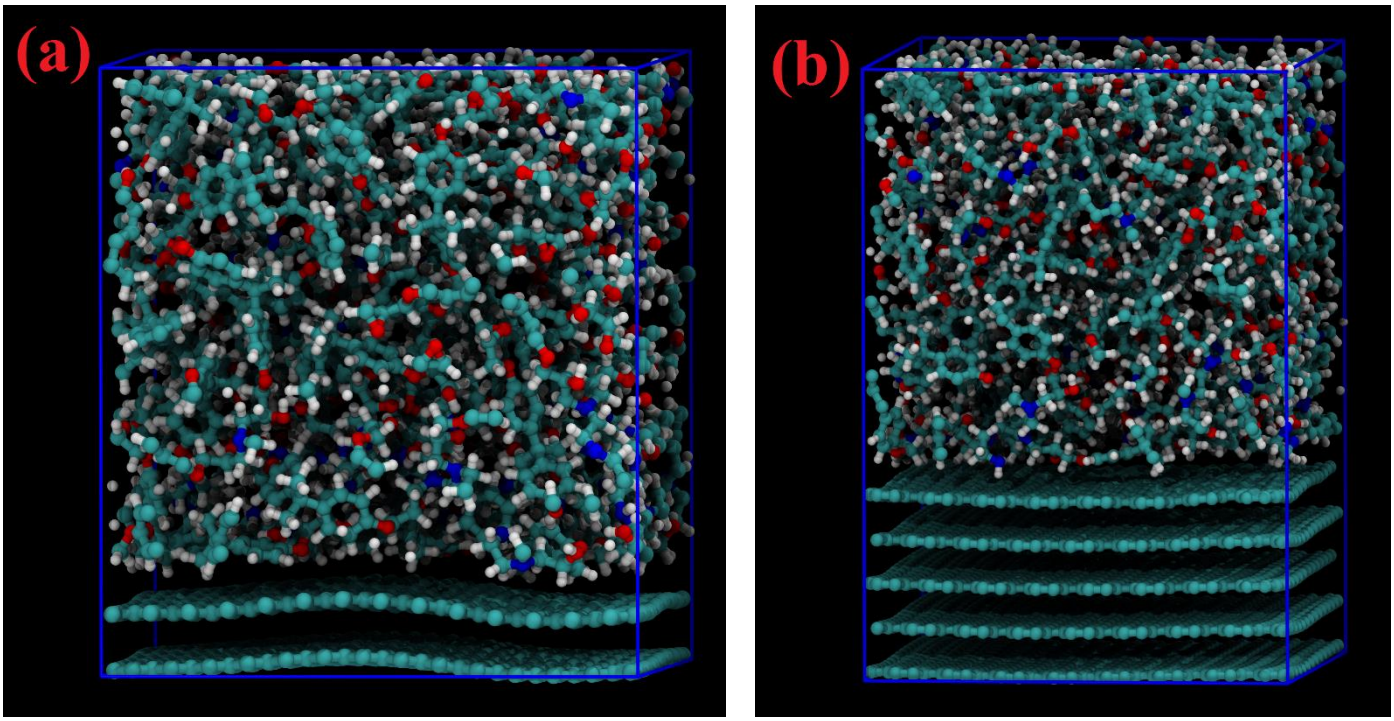

Fig. S3: Snapshots of the 80% crosslinked systems with: (a) two-layer and (b) five-layer of graphene. With the two-layer system (L2C80), the graphene layers are subjected to more deformation.

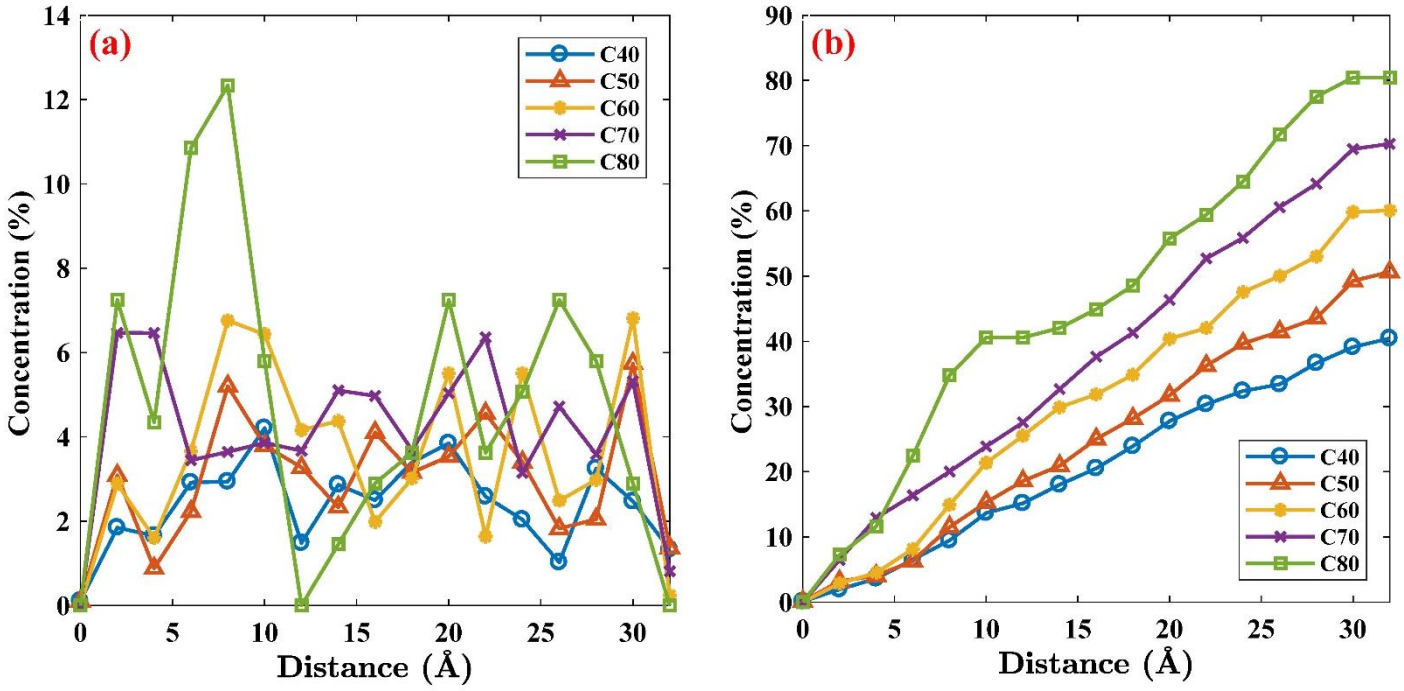

Fig. S4: Local and accumulated distribution of crosslink bonds for the five-layered graphene systems with different crosslinking densities. The accumulated distribution density profiles were plotted based on the local distribution curves from the graphene layer side (C40 to C80 denotes the crosslinking densities of 40% and 80%).

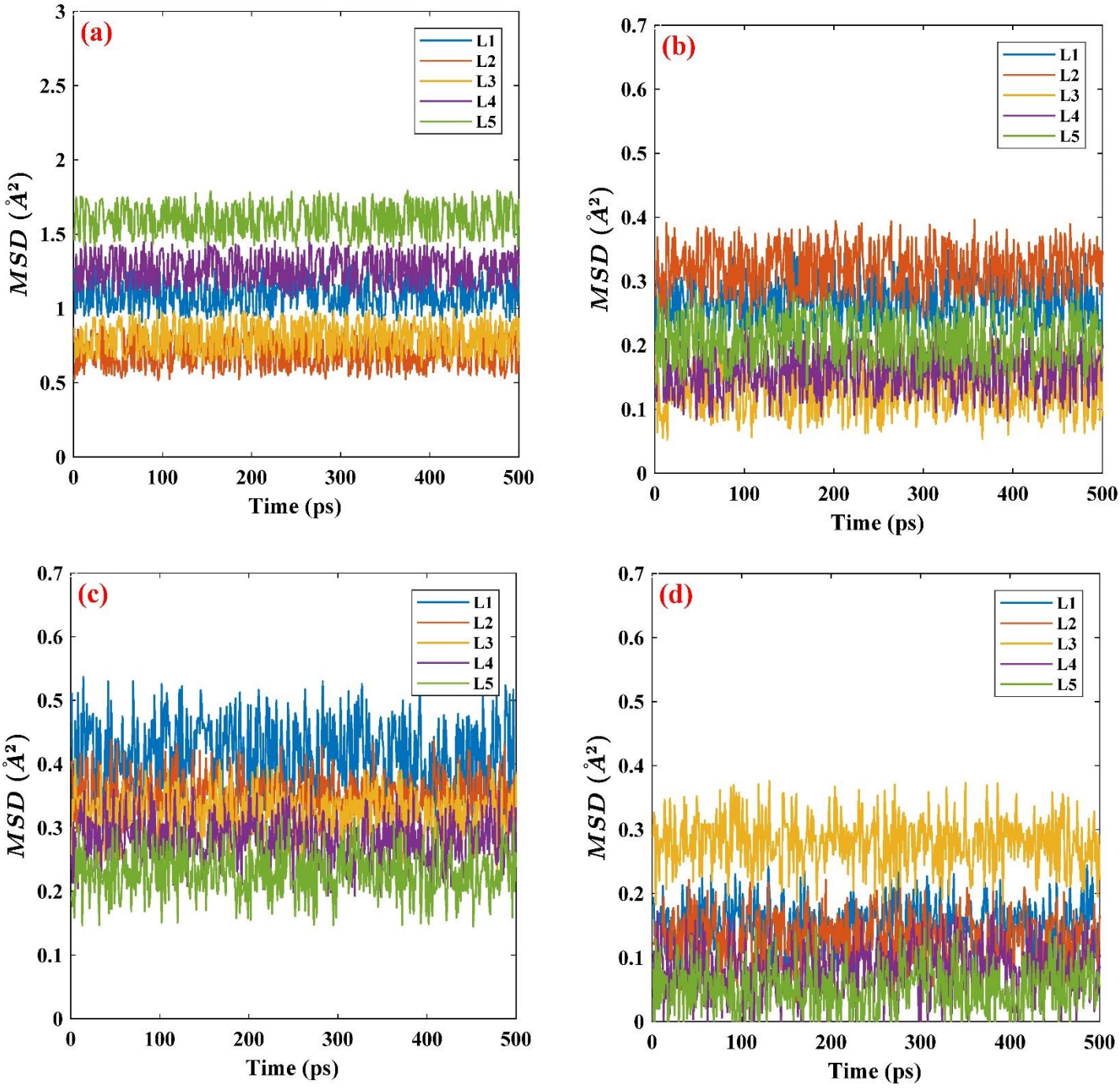

Fig. S5: Mean-squared displacement (MSD) of all atoms in the: (a) bulk region for 40% crosslinked, (b) bulk region for 80% crosslinked, (c) interphase region for 40% crosslinked, and (d) interphase region for 80% crosslinked samples with different numbers of graphene layers (L1 to L5 stands for the number of graphene layers from 1 to 5).

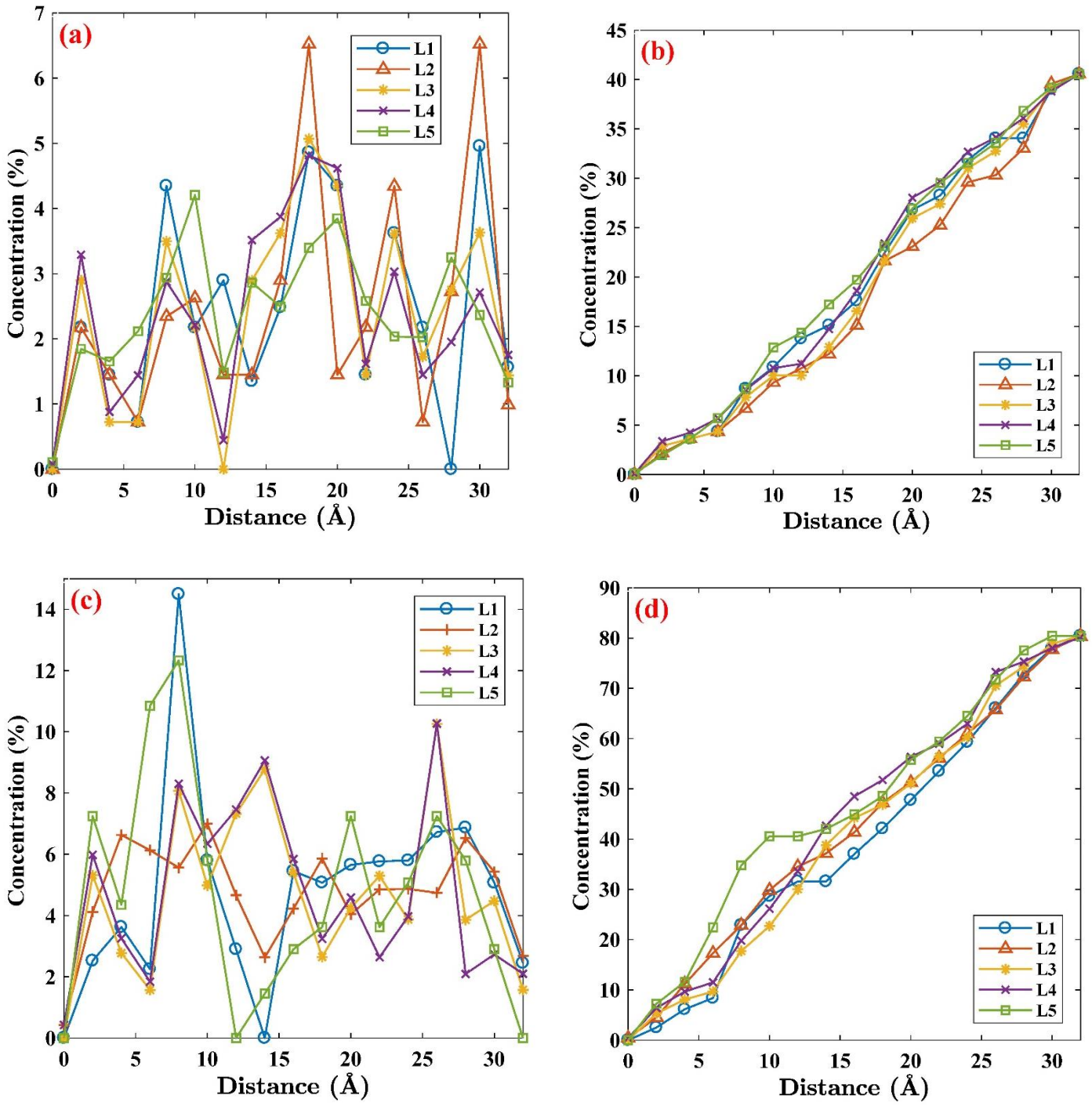

Fig. S6: Local distribution of crosslink bonds in the systems with: (a) 40% and (c) 80% crosslinked density. Accumulated distribution of crosslink bonds for: (b) 40% and (d) 80% crosslinked epoxy. The accumulated distribution density profiles were plotted based on the local distribution curves from the graphene layer side (L1 to L5 stands for the number of graphene layers from 1 to 5).

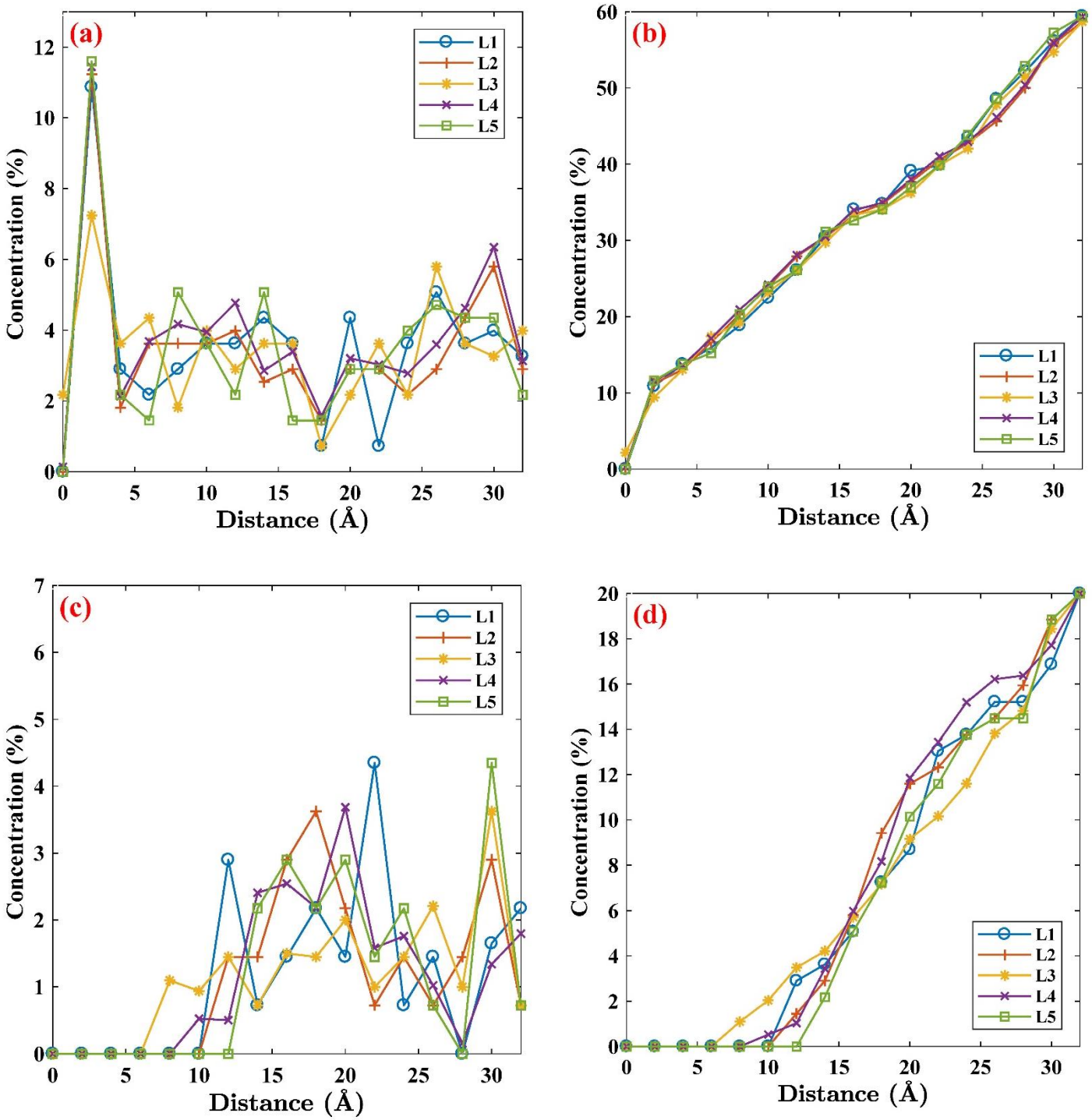

Fig. S7: Local distribution of unreacted epoxide group in the systems with: (a) 40% and (c) 80% crosslinked density. Accumulated distribution of unreacted epoxide group for: (b) 40% and (d) 80% crosslinked epoxy. The accumulated distribution density profiles were plotted based on the local distribution curves from the graphene layer side (L1 to L5 stands for the number of graphene layers from 1 to 5).

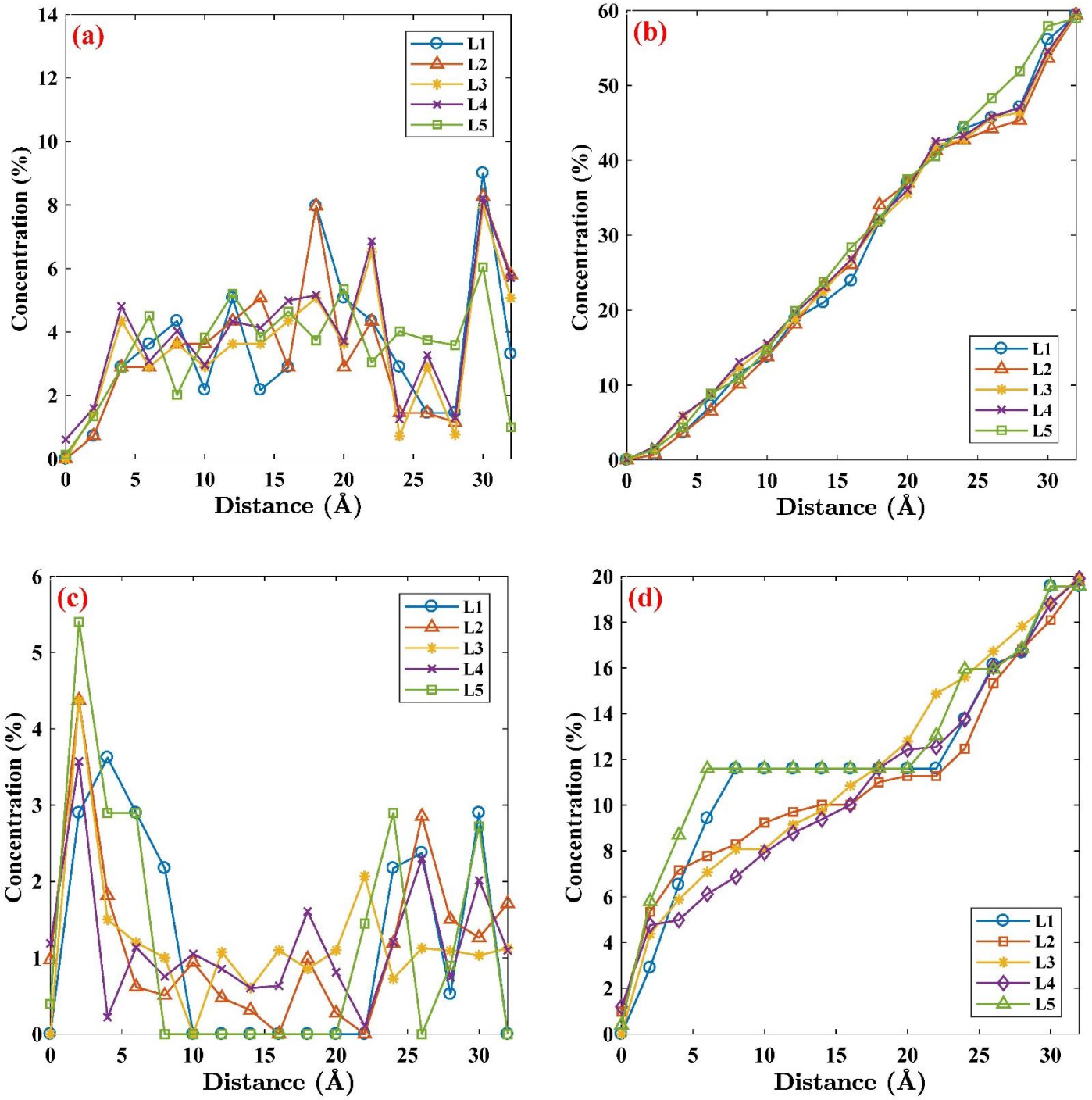

Fig. S8: Local distribution of unreacted amine group in the systems with: (a) 40% and (c) 80% crosslinked density. Accumulated distribution of unreacted amine group for: (b) 40% and (d) 80% crosslinked epoxy. The accumulated distribution density profiles were plotted based on the local distribution curves from the graphene layer side (L1 to L5 stands for the number of graphene layers from 1 to 5).

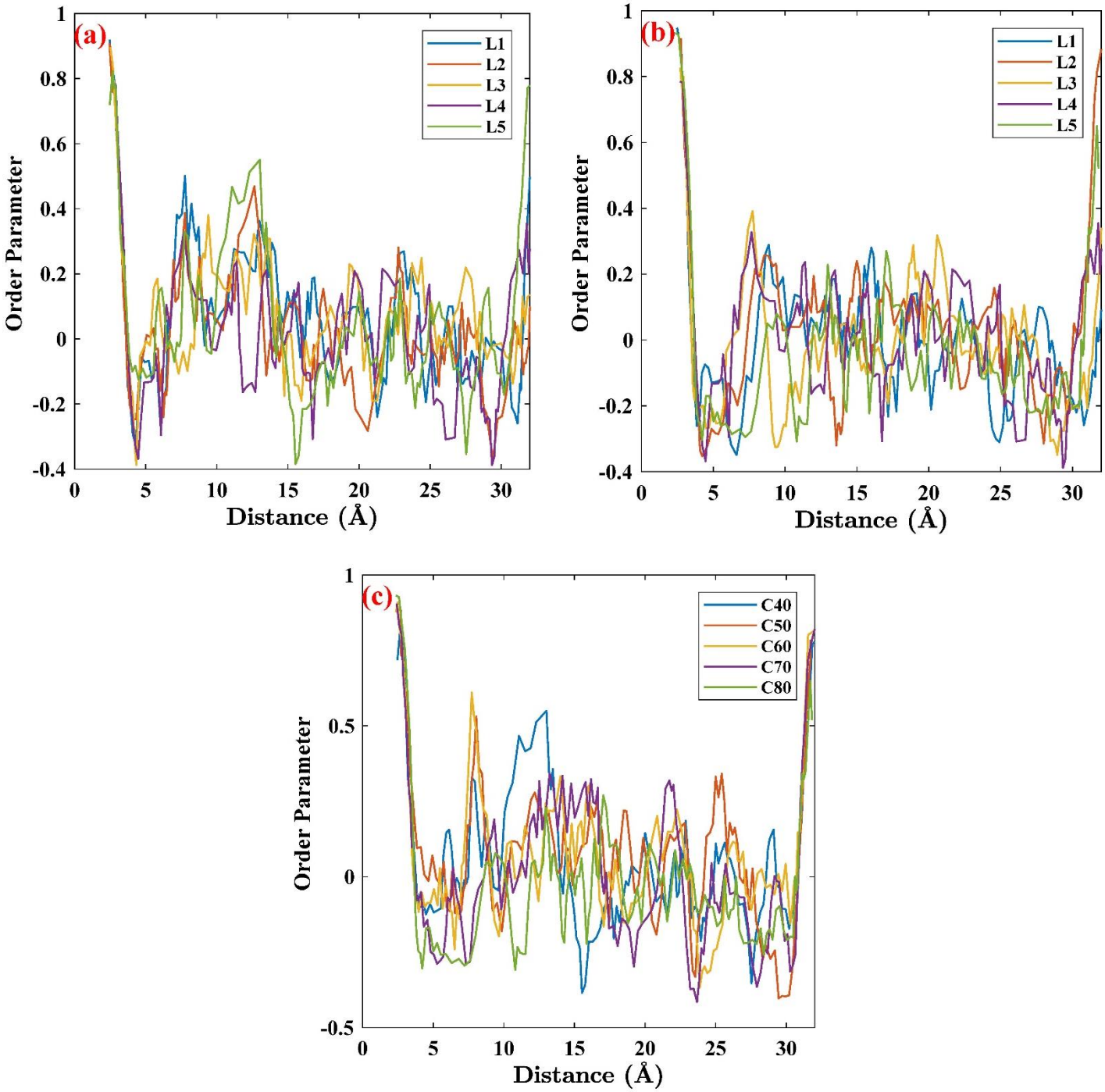

Fig. S9: Order parameter for the aromatic rings of epoxy chains as a function of the distance from the graphene surface for: a) 40% crosslinked epoxy, b) 80% crosslinked epoxy, and c) five-layer graphene systems with different crosslink densities (L1 to L5 stands for the number of graphene layers from 1 to 5, while C40 to C80 denotes the crosslinking densities of 40% and 80%).