Journal Name

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SUPPORTING INFORMATION

Melamine-exfoliated graphene aqueous dispersion: unveiling microsolvation features with density functional theory

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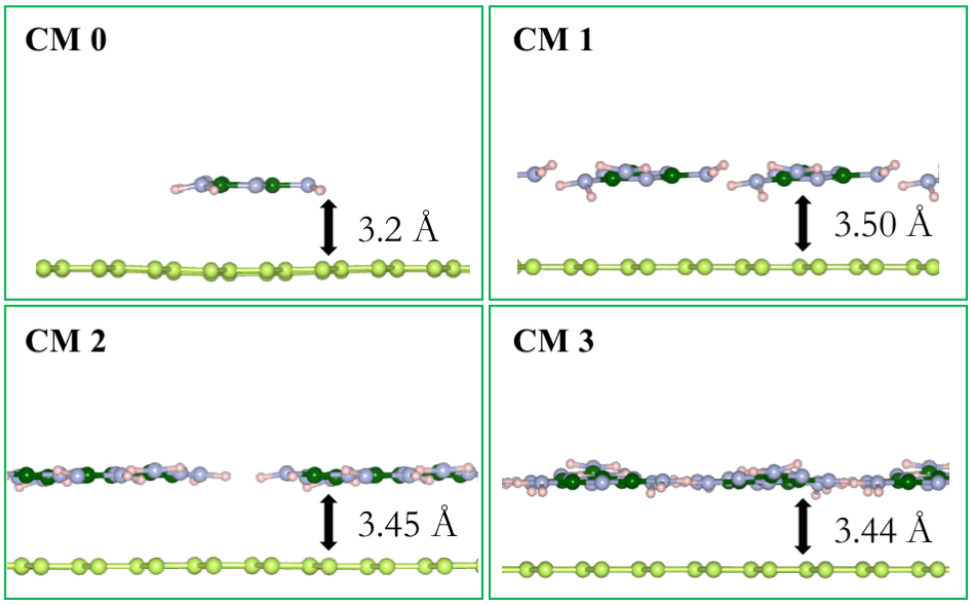

Figure S1. Side view of the minimum-energy CMx geometries obtained at the PBE-D3 level of theory.

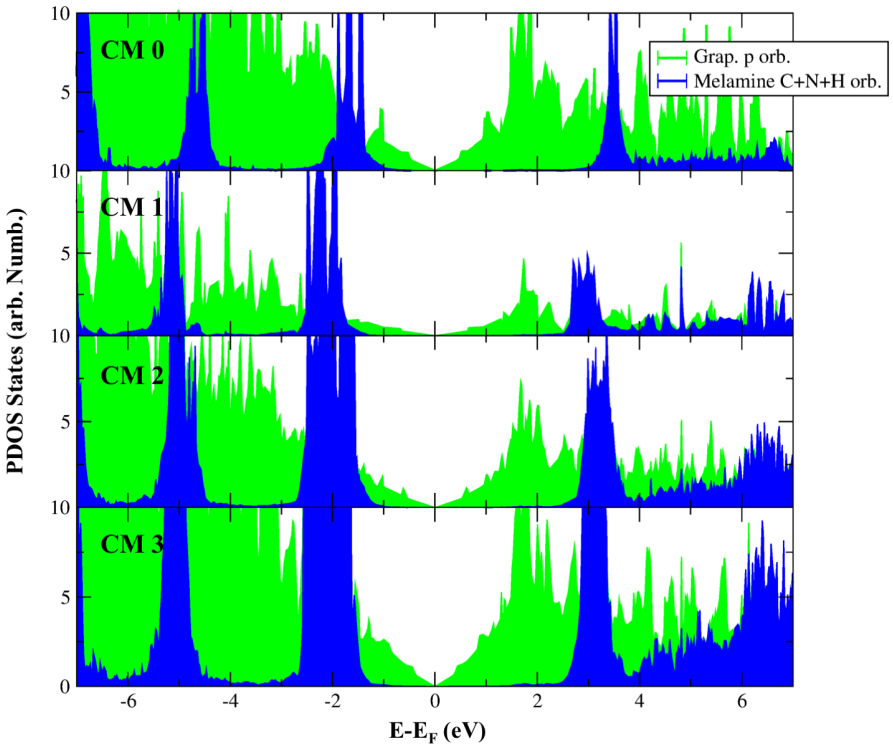

Figure S2. Partial densities of states (PDOS) at the PBE level of theory for the CMx systems. For visualization purposes, only C (p orbitals) contributions are shown for graphene and the melamine contributions are shown as the sum of the C-N-H orbitals.

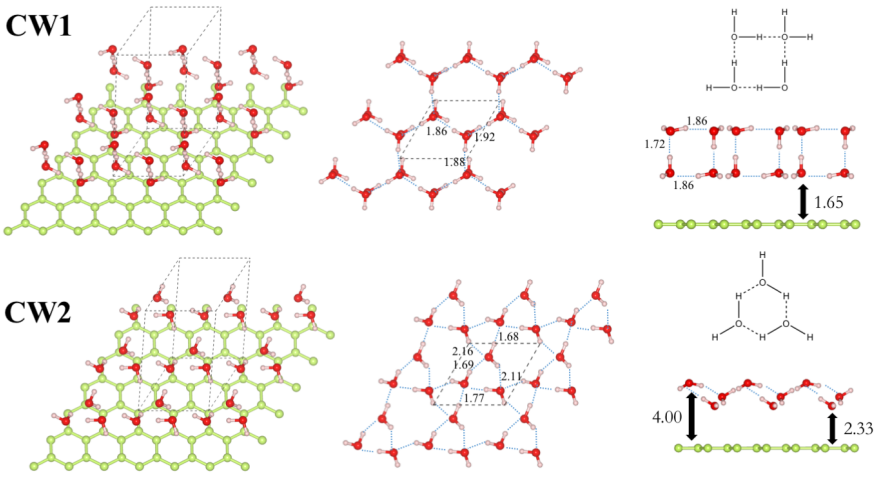

Figure S3. Geometries and structural features for the CWx systems. In all cases, distances are in angstroms.