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Effects of single adatom and Stone-Wales defects on the elastic properties of carbon nanotube/polypropylene composites: a molecular simulation study

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Highlights

- Effect of single adatom and Stone-Wales defects on longitudinal elastic properties of carbon nanotube/polypropylene composites was contrastively studied.
- Elastic properties of single adatom and Stone-Wales defected carbon nanotube/polypropylene composites strongly depend on that of individual carbon nanotubes.
- Variation in elastic properties of single adatom and Stone-Wales defected carbon nanotube/polypropylene is mainly attributed to their structural relaxation.

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