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Energy landscape of carbon nanotube caps: lack of intrinsic chirality bias and consequences for selective growth VASILII ARTYUKHOV, EVGENI PENEV, BORIS YAKOBSON, Rice University, Houston, TX 77005 — In the initial stages of carbon nanotube (CNT) growth, a fixed pattern of six pentagons encodes what unique (n, m) chirality a nascent CNT would inherit and can be viewed as its "inorganic gene". We shall present the results from a large-scale computational effort designed to establish a quantitative structure–property (intrinsic elastic energy) relation for a set of more than 4500 caps, including all isomers that obey the isolated pentagon rule, corresponding to tube diameters $d \leq 1$ nm. Our analysis shows that the energy scale associated with the CNT caps is small, compared to that of the CNT/catalyst interface. Such a flat energy landscape is irrelevant to chiral selectivity and lends further credibility to interface-controlled scenarios for selective growth of single-walled CNTs.

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