Recent advances in understanding carbon nanotube growth through atomic scale simulations

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Although growth of materials is a pre-eminently experimental area of research, computational studies in general, and atomistic simulations in particular, have contributed significantly to our understanding of the metal-catalyzed CNT growth process. Such simulations have indeed resolved many key issues and revealed a manyfold of detailed insights in the growth mechanism, including e.g. an atomistic view on carbon dissolution and surface seggregation [1, 2], carbon polyyne formation at the surface [3], and cap lift off [4, 5]. First, I shall highlight a selection of simulations which have provided such insights and demonstrate how they have contributed to our understanding of the growth process [6]. Subsequently, a number of recent efforts will be highlighted which address previously uncovered areas, including ion bombardment [7, 8], growth from hydrogen containing growth precursors [9], and the application of accelerated atomic scale techniques for studying the dynamics of the growth process [10].

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