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Polymeric CNT composites: atomistic simulations of interfacial properties JACEK GOLEBIOWSKI, ARASH A MOSTOFI, PETER D HAYNES, Imperial College London, Thomas Young Centre — Functionalized carbon nanotube (FCNT)/polymer composites have received significant interest as promising structural materials with applications in the most demanding areas of industry such as ballistic protection. In order to optimise the properties of this class of materials, it is imperative to understand how load is transferred through the FCNT-polymer interface with the aim to identify the key factors determining the interfacial shear strength and dominant failure mechanisms. Computational investigation of the interface requires simulations of 10,000s of atoms in order to accurately describe the movement of polymer chains; however, critical interfacial failure involves changes in local chemistry such as bond-breaking effects, necessitating a quantum-mechanical (QM) treatment. These issues are addressed by employing a quantum/classical hybrid simulation technique 'Learn on the Fly' [1]. In this approach, classical molecular dynamics is used to simulate the majority of the system under strain, while regions of particular interest where changes in electronic structure are likely to occur, are investigated using QM methods resulting in an accurate description of bond-breaking processes.

[1] G Csányi, T Albaret, M C Payne, A De Vita, Phys. Rev. Let. 93(17):14, 2004

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