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First-principles simulations of failure mechanisms, mechanical strength and electromechanical response

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Mechanical failure in response to external strain occurs at time scales that are usually much longer than those that are accessible to simulation. In particular, when processes leading to failure are highly activated, straight-forward molecular dynamics simulations will lead to qualitatively wrong results for both failure modes and mechanical strength. Nevertheless, judiciously chosen simulations can identify potential failure mechanisms, which can then be accurately mapped out and assessed, resulting in correct predictions of the initial modes of failure, breakage mechanisms, and strength. As an example, we will discuss simulations of the breakage of carbon nanotubes, which have been shown by first-principles calculations to be the strongest materials known. Very recently, the predictions of their stress-induced transformations and temperature-dependent failure have been spectacularly confirmed by experiments, which corroborated the key theoretical results. Nevertheless, the predicted ultimate strength is still substantially higher than the observed one, probably due to the presence of defects in as-grown samples. The simulations have also suggested avenues for forming nanotube-based electronic devices solely by mechanical transformations. In some molecular devices, e.g., those based on rotaxane, electric field and current-induced atomic transformations are the basis of device operation. For such structures, it is necessary to use open boundary conditions to account for current flow through the molecule and for the buildup of charge at the molecular interfaces. We will describe the key steps of this approach, based on linear-scaling non-equilibrium Green's function methodology, and its first applications. In collaboration with M. Buongiorno Nardelli, W. Lu, S. Wang and Q. Zhao.