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Stretching molecules under extreme tensile strain: density functional theory versus multireference methods. GARY KEDZIORA, Engility Corp., STEPHEN BARR, RAJIV BERRY, Air Force Research Lab., Materials and Manufacturing Directorate, JAMES MOLLER, Miami University, Department of Mechanical and Manufacturing Engineering, TIMOTHY BREITZMAN, Air Force Research Lab., Materials and Manufacturing Directorate — A more refined understanding of how molecules behave under extreme tensile strain is desirable for modeling fracture initiation in polymers and other mecho-chemical studies. We investigated several quantum mechanical methods for use in multiscale models of highly strained polymers where bond breaking occurs. A small set of molecules and a protocol for stretching them were used as model test systems. The results from these tests using several functionals were compared with complete active space self-consistent field results. These test systems provide unique challenges for quantum mechanical models. Quantum mechanics is required for accurate bond breaking prediction because the results are dependent on the conformation and secondary electronic structure effects such as hyperconjugation. GGA methods with unrestricted solutions to the Kohn-Sham equations provide adequate results for our purposes even though there are some minor flaws based on the spin symmetry breaking.

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