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Bond Breaking in Epoxy Systems: A Combined QM/MM Approach STEPHEN BARR, UTC, Air Force Research Laboratory, GARY KEDZIORA, Engility Corp., Air Force Research Laboratory, ALLISON ECKER, SOCHE, Air Force Research Laboratory, JAMES MOLLER, Miami University, RAJIV BERRY, TIM BREITZMAN, Air Force Research Laboratory — A novel method to combine molecular mechanics and quantum mechanics (QM/MM) is developed with the intent to accurately and efficiently account for covalent bond breaking in polymer systems. Since classical force fields cannot accurately account for bond breaking, and QM is too demanding to simulate large systems, a hybrid approach is required. In the method demonstrated here, strain is applied to the system using a classical force field. When a bond break is likely, a zone surrounding the bond is used in a QM calculation to determine which, if any, bonds break. The QM result is then used to reconstitute the system to continue the classical simulation until another QM calculation is triggered. In this way a QM calculation is only computed when and where it is needed, allowing for an efficient simulation. A key component of this method is a density functional theory (DFT) method which provides accurate forces as bonds are pulled past their breaking points. To find the best method, a number functionals are compared with high level QM calculations by pulling various small molecules, representative of epoxies, past a bond breaking event. Appropriate values for the QM zone size and the QM trigger criteria are also determined. The overall QM/MM method is then applied to an epoxy system.

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