

# Highly cross-linked epoxy networks under mechanical strain

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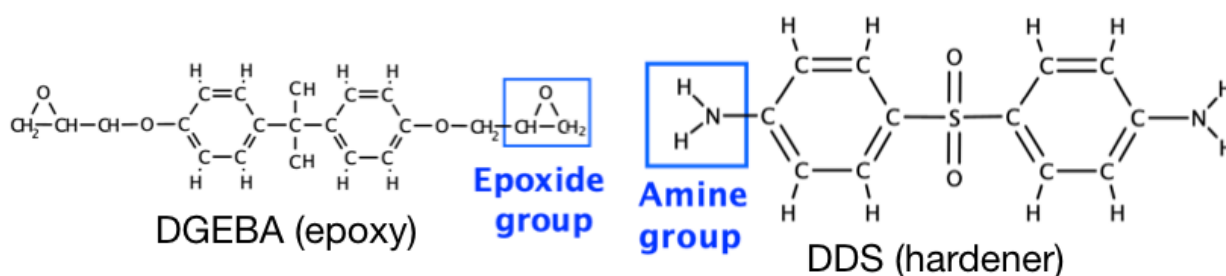
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Epoxy resins belong to a class of reactive prepolymers containing at least two epoxide groups. Thanks to their tunable properties, epoxy thermosets enjoy a breadth of applications, which shows the importance of understanding how they behave under mechanical stress. In this sense, molecular dynamics (MD) simulations can help cast light on the dynamics triggered by deformation and yield at the molecular scale.

Unfortunately, the MD description of a molecular bond, based on the harmonic potential, allows atoms to remain covalently linked at any value of bond strain, thus being unable to naturally capture bond fracture. Indeed, an accurate description of bond breakage requires quantum mechanical (QM) methods, which suffer, however, even more severe time and length scale limitations than MD does.

For this reason, combined quantum mechanics/molecular mechanics (QM/MM) approaches were developed [1], in which the bond-scission site is treated quantum mechanically, while the rest of the system is described by a much simpler and faster atomistic force-field.

This study develops a new QM/MM scheme, in which over-stretched bonds are identified by using a classical bond-length criterion, and then subject to an ONIOM [2] calculation, to decide whether or not they should break. [3,4] The ONIOM method offers the advantage of accounting for the electrostatic interaction between the QM zone and the surrounding environment, and has already been successful in modeling a number of other systems, both biological and material-based. This method will allow for the accurate modeling of highly cross-linked epoxy networks under mechanical strain.



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[2] T. Vreven, K. Suzie Byun, I. Komáromi, S. Dapprich, J. A. Montgomery, Jr., K. Morokuma and M. J. Frisch, *J. Chem. Theory Comput.*, **2006**, 2, 815-826.

[3] M. Livraghi, C. R. Wick, D. M. Smith, A.-S. Smith, *in preparation*

[4] M. Livraghi, *master thesis*, Integrated Life Sciences, FAU Erlangen-Nürnberg, **2019**