# Performance of the COMPASS force field for inorganic-organic hybrid polymers

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Inorganic-organic hybrid polymers combine inorganic and organic polymer structures in one homogenous material. Their properties can be tuned for a wide range of specific demands. Therefore these materials are of huge commercial interest. Possible applications for hybrid polymers include coatings, filling materials for dental restoration and sophisticated optical materials [1].

These hybrid polymers are synthesized in a two-step procedure, a polycondensation of the precursors – usually alkoxysilanes and/or silanols – and a subsequent polymerization of organic functionalities which are covalently bonded to the precursors. The polymerization can be initiated by two-photon absorption processes, which allows to obtain tunable microstructures with feature sizes in the 100 nm range [2,3].

Experimental results on the atomistic structures of these materials are rare, but first molecular modeling studies give a first insight [3,4]. However, extensive validation calculations are necessary to ensure proper description of the materials with a sophisticated class II force field. Until now, no validation of the thermal influence during molecular dynamics has been published.

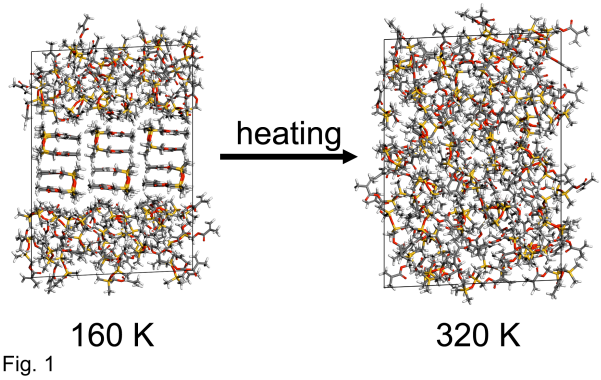


Fig. 1

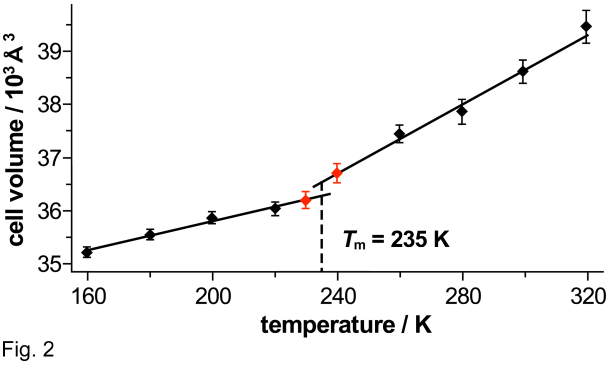


Fig. 2

The validation of the COMPASS force field [5] is performed to demonstrate the suitability of this force field for the simulation of inorganic-organic hybrid polymers. In particular, bond lengths, valence angles, and vibrational frequencies are compared for molecular structures of precursors and a small oligomer of the condensation product. The comparison with crystalline structures shows very good agreement for cell constants, symmetry, and overall structure agreement.

As the materials are usually used and evaluated under ambient conditions, their behavior during molecular dynamics is evaluated. It is shown, that densities at ambient conditions can be reproduced precisely for crystalline solids and amorphous liquids exhibiting only very small deviations. This is used for the prediction of glass transitions and melting temperatures of a small oligomer: Fig.1 shows the partially crystalline structure which is heated stepwise for the prediction of the melting temperature [6]. The resulting cell volume is depicted in Fig. 2. The melting temperature is found to be 235 K, which matches the experimental value of 238 K.

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[2] F. Burmeister et al., *J. Laser Appl.*, **2012**, *24*, 042014.
[3] F. Burmeister et al., *Optically Induced Nanostructures*, **2015**, 239–266.
[4] S. Fessel et al., *J. Sol-Gel. Sci. Technol.*, **2012**, *63*, 356–365.
[5] H. Sun, *J. Phys. Chem. B*, **1998**, *102*, 7338–7364.
[6] S.W. Watt et al., *J. Chem. Phys.*, **2004**, *121*, 9565–9573.