

# Scientific Papers

- Rheological properties of polymer chains at a copper oxide surface: Impact of the chain length, surface coverage, and grafted polymer shape  
**Phys. Rev. E** **104**, 024501 (2021); <https://doi.org/10.1103/PhysRevE.104.024501>(<https://doi.org/10.1103/PhysRevE.104.024501>)
- Strain induced crystallisation of polymers at and above the crystallisation temperature by coarse-grained simulations  
**J. Chem. Phys.** **154**, 234902 (2021); <https://doi.org/10.1063/5.0050562>(<https://doi.org/10.1063/5.0050562>)
- Assessing the derivation of time parameters from branched polymer coarse-grain model  
**J. Chem. Phys.** **154**, 124901 (2021); <https://doi.org/10.1063/5.0039843>(<https://doi.org/10.1063/5.0039843>)
- Heterogeneity Effects in Highly Cross-Linked Polymer Networks  
**Polymers** **2021**, **13(5)**, 757 (2021); <https://doi.org/10.3390/polym13050757>(<https://doi.org/10.3390/polym13050757>)
- Backbone oriented anisotropic coarse grains for efficient simulations of polymers  
**J. Chem. Phys.** **153**, 214901 (2020); <https://doi.org/10.1063/5.0019945>(<https://doi.org/10.1063/5.0019945>)
- Grain Shape Dynamics for Molecular Simulations at the Mesoscale  
**Adv. Theory Simul.** **3** **9**, 2513-0390 (2020); <https://doi.org/10.1002/adts.202000124>(<https://doi.org/10.1002/adts.202000124>)
- Development of a coarse-grain model for the description of the metal oxide-polymer interface from a bottom-up approach  
**J. Chem. Phys.** **151**, 064703 (2019); <https://doi.org/10.1063/1.5115148>(<https://doi.org/10.1063/1.5115148>)