

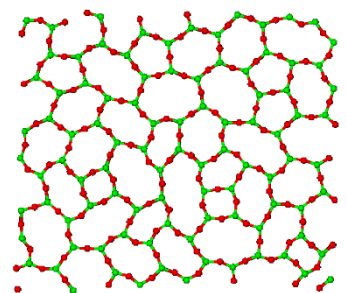
**Montag, 20.06.2016 um 17:00 Uhr**  
**Ort: Seminarraum 87, Wilhelm-Klemm-Straße 10**

## Properties of 2D silica glasses as studied by computer simulations



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The experimental progress to generate 2D silica glasses [1] [2] has offered a realistic description of the random network theory of the silica glass structure as suggested a very long time ago[3]. This extremely thin material consists of two layers of silica and exhibits 2D properties in all phases. In the glass phase, the silica network shows a log-normal ring distribution with a characteristic distribution of triplets. Two different models, based on a Soft - core Yukawa potential [4] and a Stillinger Weber type multi-body potential, have been employed for our simulations. After energy minimization, the defect free structures were identified and their ring statistics were compared with the experiment. Going beyond the experiment, the observations can be related to the underlying local energies. Furthermore, two distinct motional mechanisms can be identified which are responsible for generating local relaxation processes.



- [1] Heyde M., Shaikhutdinov S., Freund H.-J., Chem. Phys. Lett. 550, 1 (2012).
- [2] Huang P. Y. et al, Nano Lett. 12, 1081 (2012).
- [3] Zachariasen W.H., J. Am. Chem. Soc. 54, 3841 (1932).
- [4] Mendez-Maldonado G.A., et al., J. Chem. Phys. 137, 054711 (2012).