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CURRENT SESSION: Session 6: Novel Modeling of amorphous materials

PRESENTATION TYPE: Contributed (Oral)

TITLE: Ab-initio modeling of vibrational spectra of silicate glasses and decomposition into principal structural components

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Presenter Acknowledgment: I have read and acknowledge the above paragraph

ABSTRACT BODY:

Abstract Body: Density functional theory is used to calculate the vibrational properties of pure silica and sodo-silicate glasses with 20, 25, and 33 mol% of Na_2O. The infrared and Raman spectra are calculated and the full responses are decomposed into principal structural components (PSC). Those are for example the SiO_4^{n-}-tetrahedra with n non-brigding oxygens defining the Q_n-species at the origin of the structured feature at high frequency, and the Si-O-Si bridges leading the broad Raman R-band at intermediate frequencies. Our results confirm that Si-O-Si bending in bridges with large angle vibrate preferentially at lower frequencies than those with low angle. In addition, the spectral response of the Q_2-species is bimodal and overlaps with that of the Q_3, while the Q_4 response covers almost all of the spectral range of the Q_n-band. The ab-initio individual spectral responses of the PSC are used to reconstruct the experimental Raman responses. Contrary to the commonly used multi-Gaussian decomposition, this approach provides unambiguous band-assignments and hence a more accurate way to probe the structural and chemical properties of glasses from their spectroscopic signature.

KEYWORDS: ab-initio modeling, sodo-silicate glasses, vibrations, Raman.