Abstract Submitted
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Modeling vitreous silica bilayers AVISHEK KUMAR, Department of Physics, Arizona State University , MARK WILSON , Department of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford, DAVID SHERRINGTON, Department of Theoretical Physics, University of Oxford , MICHAEL THORPE, Department of Physics, Arizona State University — The recent synthesis and imaging of bilayers of vitreous silica has led to a wealth of new information [1-2]. We have modeled the experimentally-observed bilayer using a computer assembly procedure [3] to form a network of corner-sharing tetrahedra, which is then mirror-reflected to form a bilayer. We show that the vitreous silica bilayer has additional macroscopic degrees of freedom iff there is a symmetry plane through the center of the bilayer going through the central layer of oxygen ions that join the upper and lower monolayers. We have computer-refined the experimental coordinates to determine the density, and other structural characteristics such as the Si-Si pair distribution function, Si-O-Si bond angle distribution and the Aboav-Weaire law. [1] P. Y. Huang, S. Kurasch, A. Srivastava, V. Skakalova, J. Kotakoski,A. V. Krasheninnikov, R. Hovden, Q. Mao, J. C. Meyer, J. Smet,D. A. Muller, and U. Kaiser, Nano. Lett. 12, 1081 (2012). [2] M. Heyde, S. Shaikhutdinov, and J. J. Freund, Chem. Phys. Lett.550, 1 (2012). [3] M. Wilson, A. Kumar, D. Sherrington, M.F. Thorpe, Phys. Rev. B (87) 214108 (2013)

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