

Abstract Submitted  
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**Ab initio calculations of the atomic and electronic structure of crystalline  $\text{PEO}_3:\text{LiCF}_3\text{SO}_3$  electrolytes**<sup>1</sup> SHA XUE, Department of Chemical Engineering, The University of Tulsa, YINGDI LIU, HONGLI DANG, Department of Physics and Engineering Physics, The University of Tulsa, DALE TEETERS, Department of Chemistry and Biochemistry, The University of Tulsa, DANIEL CRUNKLETON, Department of Chemical Engineering, The University of Tulsa, SANWU WANG, Department of Physics and Engineering Physics, The University of Tulsa — With the advent of high conductivity polymer batteries, a great deal of research interest has been generated in the study of  $\text{PEO}:\text{LiCF}_3\text{SO}_3$  polymer electrolyte, because of its enhanced stability at the lithium/polymer interface. Experimental studies have concluded that both the  $\text{PEO}_3:\text{LiCF}_3\text{SO}_3$  crystalline complex and the  $\text{PEO}_3:\text{LiCF}_3\text{SO}_3$  amorphous phase are both present when  $\text{PEO}/\text{Li}$  ratio is greater than 3. However, most theoretical investigations to date are concerned about the short chain amorphous  $\text{PEO}:\text{LiCF}_3\text{SO}_3$  system. We report first-principles-density-functional-theory calculations of crystalline  $\text{PEO}_3:\text{LiCF}_3\text{SO}_3$ . In particular, we provide the atomic-scale characteristics and electronic structures. The calculated results about the bonding configuration, electronic structures, and conductivity properties are in good agreement with the experimental measurements.

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