Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Fast motif-network scheme for extensive exploration of complex crystal structures in silicate cathodes KAI-MING HO, XIN ZHAO, Iowa State University, SHUNQING WU, Xiamen University, XIAOBAO LV, University of Science and Technology of China, MANH CUONG NGUYEN, CAI-ZHUANG WANG, Iowa State University, ZIJING LIN, University of Science and Technology of China, ZI-ZHONG ZHU, Xiamen University — A motif-network search scheme is proposed to study the crystal structures of the dilithium/disodium transition metal orthosilicates A_2MSiO_4. Using this fast and efficient method, the structures of all six combinations with A = Li or Na and M = Mn, Fe or Co were extensively explored in this work. In addition to finding all previously reported experimental structures, we discover many other different crystal structures which are highly degenerate in energy. These tetrahedral-network-based structures can be classified into 1D, 2D and 3D types. A clear trend of the structural preference in different systems is revealed and possible indicators that affect the structure stabilities are introduced. For the case of Na systems which have been much less investigated in the literature relative to the Li systems, we predicted their ground state structures and found evidence for the existence of new structural motifs.

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Date submitted: 14 Nov 2014 Electronic form version 1.4