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Ab initio structure prediction of silicon and germanium sulfides for lithium-ion battery materials CONNIE HSUEH, Stanford University, MARTIN MAYO, ANDREW J. MORRIS, Theory of Condensed Matter, University of Cambridge — Conventional experimental-based approaches to materials discovery, which can rely heavily on trial and error, are time-intensive and costly. We discuss approaches to coupling experimental and computational techniques in order to systematize, automate, and accelerate the process of materials discovery, which is of particular relevance to developing new battery materials. We use the *ab initio* random structure searching (AIRSS) method to conduct a systematic investigation of Si–S and Ge–S binary compounds in order to search for novel materials for lithium-ion battery (LIB) anodes. AIRSS is a high-throughput, density functional theory-based approach to structure prediction which has been successful at predicting the structures of LIBs containing sulfur [1] and silicon and germanium [2]. We propose a lithiation mechanism for Li-GeS_2 anodes as well as report new, theoretically stable, layered and porous structures in the Si–S and Ge–S systems that pique experimental interest.

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