

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Silicon Framework Allotropes for Li-ion and Na-ion Batteries: New Insight for a Reversible Capacity.**<sup>1</sup> ASMA MARZOUK, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, FERNANDO SOTO, JUAN BURGOS, PERLA BALBUENA, Department of Chemical Engineering, Texas AM University, College Station, Texas, FADWA EL-MELLOUHI, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University — Silicon has the capacity to host a large amount of Li which makes it an attractive anode material despite suffering from swelling problem leading to irreversible capacity loss. The possibility of an easy extraction of Na atoms from Si<sub>24</sub>Na<sub>4</sub> [1] inspired us to adopt the Si<sub>24</sub> as an anode material for Lithium-ion and sodium-ion Batteries. Using DFT, we evaluate the specific capacity and the intercalation potential of Si<sub>24</sub> allotrope. Enhanced capacities are sought by designing a new silicon allotrope [2]. We demonstrated that these Si<sub>24</sub> allotropes show a negligible volume expansion and conserve their periodic structures after the maximum insertion/disinsertion of the ions which is crucial to prevent the capacity loss during cycling. DFT and ab-initio molecular dynamics (AIMD) studies give insights on the most probable surface adsorption and reaction sites, lithiation and sodiation, as well as initial stages of SEI formation and ionic diffusion. [1] Nat Mater 14 (2) (2015) 169 [2] Electrochimica Acta, 207 (2016) 301

<sup>1</sup>Qatar National Research Fund (QNRF) (NPRP 7-162-2-077)

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Date submitted: 03 Jan 2017

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