Nitrogen cycle in deep Earth: insights from first-principles calculations

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Important volatile elements that are key components of Earth's oceans and atmosphere are cycled through the solid Earth via tectonic processes, predominantly subduction. They pass from subducted oceanic lithosphere, through the overlying mantle wedge into volcanic systems to be emitted as gases. These volatiles are predominantly light elements, including carbon, hydrogen, helium, sulfur and nitrogen – some of the commonest elements in our galaxy. A key, unresolved question, however, is the location and concentrations of abundant volatile elements in the bulk deep Earth, their influence on solid Earth properties, and hence their influence on volcanic emissions. In particular, the origin of Earth's nitrogen-rich atmosphere is uncertain. With the development of theoretical methods and computational power, structure prediction has become possible by searching for structures with global minimal energy across an energy landscape. This is essential if we are to predict mineral hosts for nitrogen in Earth's mantle. Structure searches in the H – N – Si – O system, by evaluating the existence of phases in the NH3 – H2O – SiO2 ternary system, allow us to identify possible crystalline phases within this composition space. In the first instance we have simplified searches for volatile element bearing compounds using mineral chemical "waymarkers": for example, it is known that ammonium is approximately the same size as potassium, so potassium silicates provide a good starting point for search for ammonium-silicates.