

# Séminaire de Chimie Théorique

Salle de Réunion THEO, 3eme Est, bat. A12  
Vendredi 3 Février à 11:30

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## High pressure structure prediction and phase stability in planetary science

In this talk, I will give a brief introduction to one of the most difficult problems in the physical sciences, crystal structure prediction. I will discuss the scale of the problem, how it can be solved, and give some examples of its application in my work including the product of compressing CO and N<sub>2</sub> gases together, a new skutterudite consisting of phosphorus and nitrogen, and how it can be used in the planetary sciences to predict which phases comprise planetary cores. Finally, I will touch on the problem of how these methods can be used to build models of amorphous solids and glasses, an ongoing subject of my research.”

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