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Bibliographic project

Generation of optimized structures through Particle Swarn Optimization

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Repository: https://github.com/antoinegslr/ParticleSwarnOptimization

Introduction

Novel phases in ammonia-water mixtures under pressure

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Crystal structure prediction in Saturn and Uranus' mantles

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Novel phases in ammonia-water mixtures under pressure

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While ammonia and water readily form hydrogen-bonded molecular mixtures at ambient conditions, their miscibility under pressure is not well understood, yet crucial to model the interior of icy planets. We report here on the behavior of ammonia-water mixtures under extreme pressure conditions, based on first-principles calculations of 15 stoichiometries in the pressure range of 1 atm–10 Mbar. We show that compression facilitates proton transfer from water to ammonia in all relevant mixtures. This favors ammonia-rich hydrates above 1 Mbar, stabilized by complete de-protonation of water and the formation of the unusual structural motifs $O^{2-}\cdot(NH_4^+)_2$ and $O^{2-}\cdot(N_2H_7^+)_2$. The hydronitrogen cations persist to the highest pressures studied. We predict a new ammonia-rich 4:1-hydrate at intermediate pressures and find that by 5.5 Mbar, close to the core-mantle boundary of Neptune, all cold ammonia-water mixtures are unstable against decomposition into their constituents. *Published by AIP Publishing.* https://doi.org/10.1063/1.5063569

I. INTRODUCTION

Mixtures of molecular ices of water, ammonia, and methane (together with impurities and volatiles such as hydrogen or helium) make up a large proportion of the mantle regions of the "ice giants" Uranus and Neptune as well as large icy moons in our solar system and are presumed to feature prominently in the large number of Neptune-like exoplanets discovered by recent and ongoing astronomical observation campaigns.[1–5] It is not clear how molecular ices organize themselves inside these planetary bodies—whether they form segregated layers with distinct chemical and density profiles or homogeneous mixtures corresponding roughly to the global composition ratio throughout. High pressure conditions (which reach hundreds of GPa, or several Mbar, inside ice giants) can, in general, favor unexpected chemical motifs and thus stabilize unusual compounds and stoichiometries, as found among prototypical mineral compounds[6–10] as well as individual ices.[11–16]

The molecular ices exhibit very different chemical responses to pressure: water ice forms a sequence of atomic networks above 65 GPa, where water molecules readily give up their protons to sit at the mid-points of nearest-neighbor O–O separations,[13,14,17,18] while ammonia holds onto its protons much better and instead self-ionizes above 120 GPa into ammonium amide over a large pressure range before (in calculations) returning to packing of neutral molecules.[15,16,19] The *mixtures* of the molecular ices can feature surprising pathways to stability under compression; for instance, methane's solubility in water increases to about 40% at pressures as low as a few GPa,[20] which is largely unexplained. Mixtures of ammonia and water are of particular interest as they can form hydrogen-bonded networks. First-principles calculations have so far proven very useful in establishing or confirming the phase diagrams and properties of the individual ices and of a select few hydrate phases. Here, we present a computational study of the entire binary ammonia-water phase diagram that considers *all* mutual formation and decomposition reactions at various pressures and temperatures and also establishes which *new* hydrate stoichiometries should be stabilized under particular conditions.

II. COMPUTATIONAL METHODOLOGY

Solid crystalline structures were searched for using the particle swarm optimization algorithm as implemented in CALYPSO (crystal structure analysis by particle swarm optimization).[21,22] Structure predictions were performed with up to 16 formula units of $(H_2O)_X(NH_3)_Y$, where X and Y are integers, and at 5, 10, 20, 30, 50, 80, and 100–1000 GPa in increments of 100 GPa. These searches were performed for the three canonical ammonia-water mixing ratios. At 50, 100, and 300 GPa, binary searches were performed to look for other stable mixing ratios. If a new mixing ratio was found to be stable, further searches were performed for this stoichiometry at relevant pressures. Structure predictions at pressures over 1 TPa and up to 5 TPa failed to find any structures stable against decomposition into NH_3 and H_2O. The predicted decomposition of NH_3 above 460 GPa was taken into account throughout.[23]

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Introduction

Crystal structure prediction requires **sampling** of multiple structures

Some existing methods:

- Monte Carlo
- Simulated annealing
- Minima/basin hopping
- Metadynamics
- Genetic algorithm

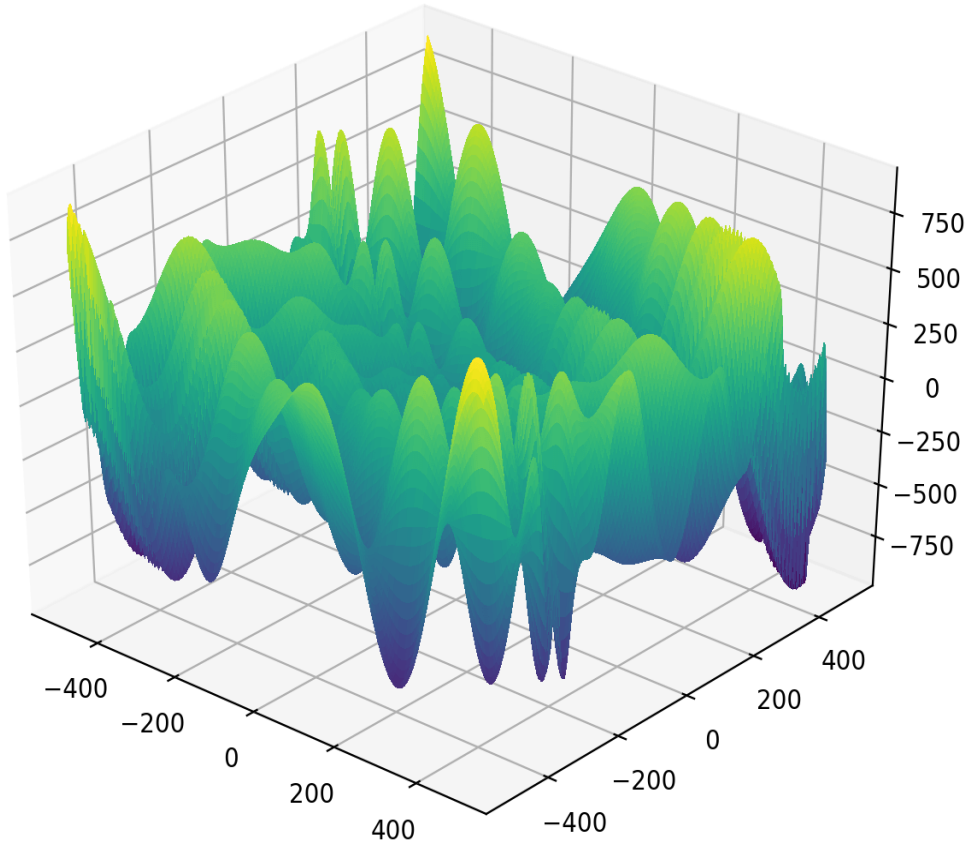

Figure 1: Eggholder function (Nathan Rooy on GitHub)

Introduction

Crystals in Saturn and Uranus:

- Presence of water ices and ammonia in similar quantities
- High pressures and temperatures

Problems using previous methods:

- High computational cost
- High energetic barriers to cross
- Has everything been sampled?
- Everything is unknown

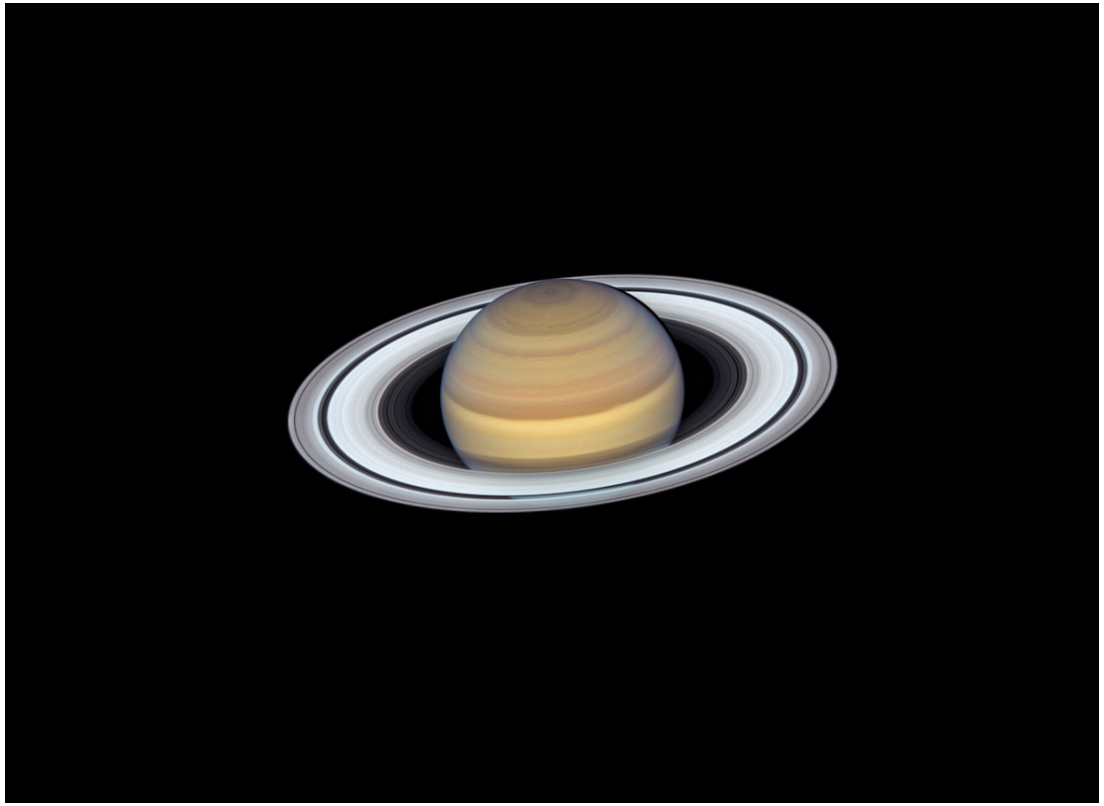

Figure 2: Saturn by Hubble telescope (Nasa, September 2019)

Particle Swarn Optimization (PSO)

> Population-based optimization algorithm based on behaviors of birds in a flock

Figure 3: Bird flock, by ...

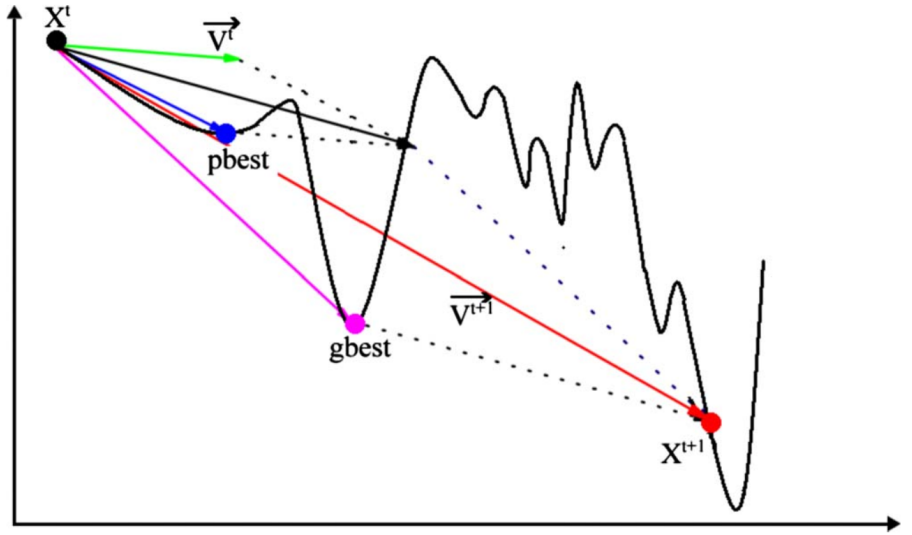

Figure 4: PSO principle, by ...

$$v_{i,j}^{t+1} = \omega v_{i,j}^{t} + c_1 r_1 (\mathtt{pbest}_{i,j}^{t} - x_{i,j}^{t}) + c_2 r_2 (\mathtt{gbest}_{i,j}^{t} - x_{i,j}^{t})$$

How does it work?

- Generation of one random structure per symmetry
- Local optimization of every structure
- Exclusion of similar structures *(through bond characterization matrix)*
- Generation of new structures by PSO, using personal and flock's hystories (global best minimum `gbest` and personnal best minimum `pbest`)
- Repetition of the three last steps until convergence (difference between two consecutive minimal values less than a defined epsilon)

> The program then returns the configuration associated to the lowest energy

PSO for crystal structure prediction

Results from previous studies

Bref voilà dire que y'avait des trucs, avec trois phases et tout

PSO for crystal structure prediction

Et là paf dire ô combien cette méthode est magique pour les trois phases : découverte de nouvelles phases avec peu d'itérations

PSO for crystal structure prediction

Slide 1: Introduction

Definition: Particle Swarm Optimization (PSO) is a population-based optimization algorithm that simulates the social behavior of birds or insects, such as flocking or swarming.
Objective: The goal of PSO is to find the optimal solution to a given optimization problem, such as finding the minimum or maximum of a function, or the best configuration of a system.

Slide 2: How it works

Each "particle" in the swarm represents a potential solution to the optimization problem.
The particles move through the solution space and update their position based on their own experience and the experience of other particles.
The position of each particle is updated using a velocity vector, which is influenced by the particle's current position, the best position it has found so far (called the "personal best"), and the best position found by the entire swarm (called the "global best").
The velocity and position updates are performed iteratively until a satisfactory solution is found or a predetermined number of iterations is reached.

Slide 3: Advantages and disadvantages

Advantages:

PSO is simple to implement, has few parameters to tune, and can handle large and complex optimization problems. It is also robust and can find good solutions quickly.

Disadvantages:

PSO is sensitive to the initial positions of the particles and can get stuck in local optima. It may also require more computational resources compared to some other optimization algorithms.

Slide 4: Applications

PSO has been applied to various fields, including engineering, computer science, finance, and biology. Some examples of problems that have been solved using PSO include:

- Function optimization
- Feature selection
- Clustering
- Neural network training
- Scheduling
- Control
- Data mining

Slide 5: Conclusion

In summary, PSO is a powerful and versatile optimization algorithm that can find good solutions to a wide range of problems. However, it may not always be the best choice for every problem, and it is important to consider the trade-offs and limitations of using PSO.