# Inside Neptune-like Planets from First Principles

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## Introduction

Over the past decade, nearly two thousand confirmed exoplanets have been discovered, along with five thousand candidate ones. Of these, there have been an unexpectedly large number that are Neptune-like.

For Uranus and Neptune, two different interior models have been constructed:

- A (traditional) "three-layer model": a core made of "rocks" (silicates and iron), an "icy" shell ($H_2O$, $CH_4$, $NH_3$, and $H_2S$), and a gaseous envelope ($H_2$ and He)[1]
- A single layer of H and He, with a compositional gradient of heavier materials (e.g., $H_2O$ or $SiO_2$)[2]

Recent calculations[3] suggest that homogeneous mixtures (liquid) of $H_2O$ and $H_2$ are thermodynamically preferred for all concentrations from 2–70 GPa and 1000–6000 K. This supports the second model, meaning that the interior structures of such planets are poorly understood.

Previous calculations[4] have assumed icy shells of pure $H_2O$. Given the abundance of $H_2$, and that no phase separation is expected (in the liquid), it is important to consider the possibility of mixed solid phases.

**Our objective was to determine the thermodynamic stability of solid $(H_2O)_{1-x}+(H_2)_x$ phases at planetary conditions.**

## Methods

**We performed exhaustive searches for thermodynamically-stable compositions, and analyzed their properties.**

Our approach:

1. Identify candidate structures
2. Determine ground-state structures
3. Determine compositional stabilities
4. Calculate finite-temperature effects

We considered:

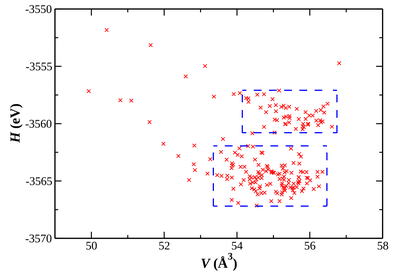
- Pressures: 0 to above 500 GPa
- Relative compositions: 1:4 to 4:1 $H_2O$:$H_2$

All calculations were performed using density-functional theory.

## Candidate Structures

**Candidate structures were identified, by performing *ab initio* random structure searching[5].**

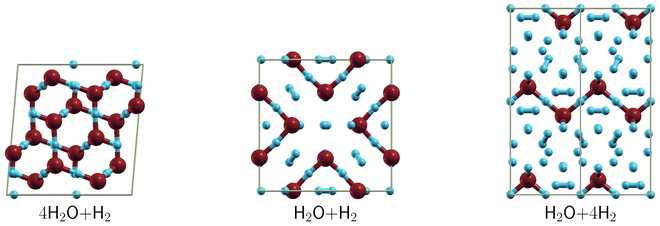
**Example:** Random trials for $6H_2O+2H_2$ at 200 GPa




## Ground-State Structures

**Ground-state structures were determined, by calculating zero-temperature phase diagrams.**

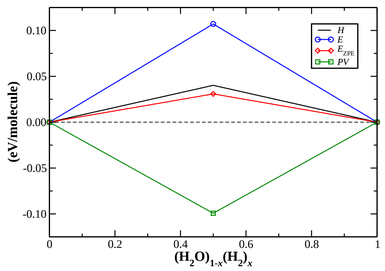
**Example:** Ground-state structures at 200 GPa




## Compositional Stabilities

**Stabilities toward decomposition were determined, by calculating energies of formation.**

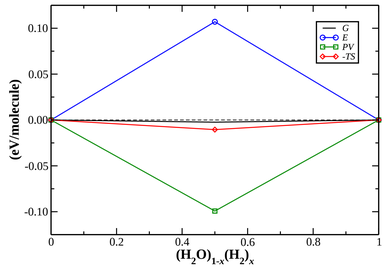
**Example:** Energies of formation at 200 GPa and 0 K




## Finite-Temperature Effects

**Energies of formation at finite-temperature were calculated, using the quasiharmonic approximation.**

**Example:** Energies of formation at 200 GPa and 4250 K




## Summary and Future Work

**Summary:**

- $(H_2O)_{1-x}+(H_2)_x$ exhibits a rich phase diagram
- At 0 K, mixed phases are marginally unstable ...
- ... but at planetary temperatures, they are stabilized by vibrational entropy

**Future work:**

- Accurate resolution of the small differences in energies
- Finite-temperature properties (e.g., superionicity)
- Other material compositions

## Acknowledgments

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## References

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