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The sky is made of lava: how lava worlds reveal their interiors through their atmospheres

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ENGLISH SUMMARY

In the past 30 years, exoplanet science has evolved exponentially. Since the discovery of the first exoplanets in the 1990s, we have progressed from mere detection to the physical and chemical characterization of these distant worlds through observations of their spectra. The niche of "hot rocky exoplanets" (HREs) is promising the potential of offering a unique window into rocky planet compositions atmosphere and interior compositions. Potentially providing valuable new information for developing our understanding of planetary formation, differentiation, and atmospheric evolution.

HREs are short-period rocky planets with dayside equilibrium temperatures in excess of 1500 K, high enough to melt rock and to support oceans of lava on their daysides, and potentially also their nightsides. These lava oceans create a direct interface between a planet's interior and atmosphere, allowing for the possibility of probing the interior composition of these planets remotely, by interpreting the spectral features shaped by chemical exchange between the melt and the atmosphere. Unlocking this potential demands comprehensive modelling approaches that account for the diverse physical and chemical processes operating within these planets. One these processes in particular is that of the vaporisation of the lava on the surface of a planet and how changing its composition affects the atmospheric composition of the planet and hence its spectral signature.

The primary goal of this thesis is to develop such models, enabling the simulation of vapor atmospheres above magma oceans under a wide range of physical and chemical conditions. To this end, I developed LavAtmos, an open-source code that calculates the equilibrium chemical composition of the vapor above a silicate melt at given temperatures, pressure, and melt composition. When we include this code within a broader modelling framework that includes atmospheric chemistry and radiative transfer calculations, it allows for the generation of self-consistent synthetic spectra for hot rocky exoplanets. The work presented in this thesis focuses on the development of LavAtmos, its implementation in the broader modelling framework, and the resulting implications for HRE science.

Chapter 2 of this thesis introduces the development and validation of the LavAtmos code in its first form, focusing on "dry" systems - those that exclude volatile-bearing species. LavAtmos calculates the chemical equilibrium between a melt and its vapor phase by combining thermodynamic data from MELTS with and internally consistent calculation of O_2 partial pressure, constrained by both the law of mass action and mass conservation. This approach allows us to determine the gas-phase abundances of over 50 chemical species, given an input silicate melt composition and thermodynamic state. LavAtmos is validated through comparison with the (relatively sparse) available experimental data as well as with other published vaporisation models.

In Chapter 3, we implement LavAtmos in the broader physical and chemical framework so as to enable us to explore how variations in bulk composition

of the magma ocean influence the observable emission spectra of HREs. This is a key question to answer for interpreting data gathered using the recently launched JWST, which has, and will continue to, target many of these worlds in its observation cycles. This study focuses specifically on how the abundances of major oxides in the melt - such as TiO_2 , SiO_2 , Na_2O , and K_2O - affect atmospheric chemistry and radiative properties. The modelling framework includes an equilibrium gas-chemistry code and a radiative transfer code to self-consistently compute atmospheric temperature-pressure profiles and emission spectra.

We find that although many melt composition changes have relatively minor spectral consequences, a few compositions stand out. High TiO_2 content in the melt increases atmospheric TiO abundances, which, due to its strong short-wave opacity, has a strong influence on the surface temperature and the emission spectra of HREs. This creates a degeneracy with heat-redistribution efficiency, which may potentially be broken by observing the optical TiO emission feature. SiO_2 also exhibits noticeable effects on the atmospheric spectrum, particularly in enhancing the SiO and SiO_2 features. The alkali oxides (Na_2O , K_2O) primarily influence surface pressure and secondary gas-phase abundances but have less direct spectral impact.

While Chapters 2 and 3 focus on volatile-free ("dry") modelling, Chapter 4 acknowledges a limitation of that approach. Recent observations and theoretical studies suggest that HREs, despite their high temperatures, may be able to host volatile-bearing atmospheres containing elements such as hydrogen, carbon, nitrogen, sulphur, and phosphorus. To address this, we developed LavAtmos 2, an upgraded version of the original code that includes volatile species in the melt-vapor equilibrium calculations. Again using the dual constraints of mass action and mass conservation to constrain the O_2 partial pressure, we calculate the composition of the vapor above a melt in a system containing both melt species and volatile elements. Incorporating an existing gas-chemical equilibrium code named FastChem allowed us to expand the number of considered gas phases to 523.

Using this model, we investigated idealized atmospheres containing only a single volatile element, more realistic "complex" volatile atmospheres containing all five tested volatile elements, and two different potential atmospheric volatile compositions for 55-Cnc e. The inclusion of volatiles was found to significantly increase the partial pressure of major gas species such as SiO , SiO_2 , Na , and K when compared to dry cases. It also led to a much higher abundance of Oxygen in the atmosphere, which in turn enhanced the abundance of key volatile species such as CO_2 and H_2O . These changes have direct implications for observable spectra and could serve as diagnostic signatures for the presence of volatiles and potentially even surface lava oceans.

In the final chapter of this thesis, we treat the radiative consequences of including volatile species - particularly hydrogen - in HRE atmospheres. One of the most important opacity sources in high-temperature, hydrogen-bearing

atmospheres is the H^- ion. Known to dominate the continuum opacity in stars and hot gas giants, H^- can significantly reshape the thermal emission spectrum of a planet if free electrons are abundant. Through the application of the modelling framework from Chapter 4, we investigated the impact of H^- opacity in HREs with varying atmospheric H abundances.

We show that even at H volume mixing ratios as low as 10^{-5} , planets with surface temperatures above 2500 K exhibit strong H^- continuum absorption, sufficient to dominate over molecular features such as those from H_2O and SiO . This happens thanks to the ionisation of alkali metals at high temperatures which supplies the free electrons needed for H^- absorption to occur. The result is a suppression of spectral lines and a smoother, more blackbody-like emission spectrum. This effect makes atmospheric retrieval more difficult, as it weakens or erases the distinct molecular features typically used for compositional analysis. However, the presence of a strong H^- continuum itself may be a clue: its strength implies a high abundance of free electrons, which in turn may point to the existence of a hot, molten, metal-rich surface interacting with a hydrogen-bearing atmosphere.

In summary, this thesis provides a comprehensive framework for understanding the chemical and radiative behaviour of hot rocky exoplanets, from the fundamental processes of lava vaporization to the observational signatures potentially detectable with modern space telescopes. By developing and applying LavAtmos, both in dry and volatile-including atmosphere, this work offers new insights into how surface and atmospheric compositions are linked, and how these links manifest in planetary spectra. These models can be used for interpreting forthcoming data from JWST and future missions, and offer a roadmap for inferring interior properties of rocky exoplanets through remote atmospheric characterization. As observations continue to improve, the tools and findings developed here will hopefully be off use in unravelling the complex processes that shape some of the most extreme terrestrial planets in the galaxy.