**Geophysical insights into the thermochemical evolution of Mars' deep interior with InSight 2018**

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NASA's InSight Mission (Banerdt et al., 2012) is due to land on Mars at the end of 2018. It aims to place new constraints on Mars' internal structure, which will in turn allow us to investigate planetary formation and Solar System evolution. InSight will determine Mars' internal structure using seismic travel times and waveforms (Phillips and Grimm, 1991; Teanby, 2015) recorded by VBB and SP seismometers (the SEIS experiment; Lognonne et al., 2014), by using a heat flow probe (HP3; Spohn et al., 2012) to constrain the thermal gradient in the uppermost lithosphere and by accurately measuring nutations due to the core with an X-band RADAR instrument (RISE; Folkner et al., 2012). These measurements will give us unprecedented constraints on the size and density of the core and on seismic velocities through the planet.

In order to interpret the data returned from the InSight Mission in terms of internal structure, temperature, chemistry and formation, it is imperative that we have accurate thermodynamic and thermoelastic models of silicates and metallic/sulfidic melts. Currently, thermodynamic and thermoelastic models used in planetary modelling ignore the effects of ferric iron and partitioning of iron between silicate minerals and sulfides. Despite reducing conditions in the interior, high pressures are expected to stabilise ferric iron, fundamentally changing the phase relations in the deep mantle. A second poorly understood phenomenon is the effect sulfur has on the high pressure partitioning of trace elements between metallic and silicate melts, a key geochemical constraint for core formation models. Without improvements in our understanding of these key processes, it will be impossible to accurately interpret geophysical data from Mars in terms of the evolution and present day state of its interior, one of the key aims of the InSight Mission.

**Using a combination of lab experiments, thermochemical and seismic modelling, and seismic data interpretation this project will enable us to create self-consistent interpretations of Mars' internal structure. This will be achieved by the following key aims:**

**(1) High pressure experiments to determine the role of iron autoredox reactions under conditions appropriate for Mars' interior. Previous work on Martian compositions has not considered these reactions, which are known to be extremely important on Earth.**

**(2) High pressure experiments to isolate the effect of silicate melt composition on high pressure partitioning of trace elements. Such data will be required to interpret the density and seismic velocities in Mars' core in terms of existing geochemical data from Martian meteorites.**

**(3) Creation of thermodynamic/thermoelastic models of minerals and melts existing in the deep mantle and core of Mars. These thermodynamic models are necessary to model seismic velocities in the deep interior as a function of pressure and temperature.**

**(4) Geophysical modelling of Mars using InSight data, including an assessment of parameter trade-offs and uncertainties. This will be vital to produce models of Mars' interior from limited seismic data recorded by a single seismometer, which will be especially important in the first few months after the deployment of the SEIS experiment.**

These additions to our understanding will be used in conjunction with InSight data to fulfil major mission goals, constraining the thermochemical structure of the deep interior and the formation of the planet over 4.5 billion years ago.

**(WP1)** **The ferric iron content and composition of sulfide in Mars' deep mantle**

**At pressures above ~6 GPa (600 km in Mars), Fe3+ becomes an important constituent in mantle phases (e.g. Frost et al., 2004, Rohrbach et al., 2007). To maintain charge balance, Fe0 enters a metal phase or sulfide melt. Although this effect is well accepted, there is very little data on the magnitude of this effect as a function of P, T and chemical composition, without which it is impossible to calculate mineral and melt phase equilibria in Mars' deep interior. These equilibria determine densities and seismic velocities, and therefore ignoring the presence of sulfide melt and Fe3+ in silicate phases could have a large effect on interior structure models. In this work package, I will conduct high pressure laboratory experiments to better quantify the effect of pressure and temperature on the redox state of iron in majoritic garnet under Mars-like conditions. The results will be combined with the few experimental data from the literature to create a thermodynamic solution model for garnets, which can be easily incorporated into software which calculates densities and seismic velocities as a function of P and T, and which informs models of Mars' interior.**

The disproportionation of iron in Mars' deep mantle can be described by the following autoredox reaction:

3Fe2SiO4 (e.g. ringwoodite) = Fe3Fe2Si3O12 (garnet) + Fe (metallic/sulfidic)

In the Earth, garnet can accommodate over 25% iron as Fe3+ at 14 GPa (Rohrbach et al., 2007; 2011). On Mars, iron contents are much higher than on Earth (Mg# ~ 75; Wanke and Dreibus, 1994), and the mantle is believed to contain markedly more sulfide (~6000 wt ppm FeS; Tuff et al., 2013). As a result, autoredox is likely to be at least as important on Mars as on Earth, despite highly reducing conditions at the surface. Because of the major effect of autoredox on the compositions and properties of both silicate and sulfide phases, it is vitally important to quantify the magnitude of the effect.

In this study, I will conduct multi-anvil experiments at high pressure with Mars-like mantle compositions in order to determine the effect of P, T and iron fugacity on Fe3+ in garnet. Experiments will be run in a 10/4 assembly (Figure XXXX) at pressures corresponding to Mars' mid-to-lowermost mantle (14, 17 and 20 GPa), and at temperatures of 1600-1900 °C. Iron or metal-metal oxides will be used to buffer the iron and oxygen fugacity of the system via the equilibrium (Stagno et al., 2013):

2Fe2SiO4 + 2Mg2SiO4 (ringwoodite) = Mg4Si4O12 (garnet) + 8Fe + 4O2

Recovered phases will be analysed for ferric iron content via Mössbauer spectroscopy.

*Figure XXXX: a) Multi-anvil assembly. b) Back-scattered electron image of a recovered charge from a multi-anvil run, showing precipitation of metallic iron and the presence of ferric-iron bearing silicates.*

Using the data obtained from this work package, and an estimate of bulk composition and sulfur content, it will be possible to calculate the amount of ferric iron and composition of sulfide in the Martian mantle as a function of pressure. I will use these new data as input to interior structure models, such that they can output the speciation of iron within mineral and sulfide phases throughout the mantle, and the resultant densities and seismic velocities. I will also compare the sulfide composition of the mantle with estimates of sulfur in the core.

**(WP2) The effect of mantle composition on partitioning of elements during core formation on Mars**

**The formation of Mars' core was facilitated by large scale melting of the mantle induced by dissipation of gravitational energy from impacts and energy from short-lived radionuclides. The last time the material in the core equilibrated with silicate material was probably within these magma oceans (e.g. Deguen et al., 2014). For this reason, it should be possible to use information from trace element partitioning between silicate and metallic/sulfidic melts to constrain the conditions of mantle-core equilibration, and therefore the composition of the core (e.g. Rubie et al., 2015). Currently missing are robust constraints on the effect of silicate composition on trace element partitioning (see Righter et al., 2016). This is particularly important for elements with high valence states, such as W, Mo, Ta and Nb. In this work package, I will take a novel experimental approach inspired by the modelling of Wood and Wade (2013). Silicate melts with different compositions will be equilibrated with nominally pure siderophile metals (W, Mo, Ta, Nb) at fixed pressure and temperature. The concentrations of these elements will be measured with LA-ICP-MS to constrain the activity coefficients in the metals. The results will then be combined with literature data to create models for trace element incorporation that can then be used to match geochemical observations with models of Mars' formation. Of particular interest will be the effects of fractionation in the magma chamber and light element concentration in the core. The effects of magma chamber fractionation might still be present and geophysically observable in Mars' mantle (Elkins-Tanton et al., 2003), and the light element concentration of the core will also be compared with or jointly inverted with geophysical estimates (see WP3; Badro et al., 2015) from the InSight Mission.**

In this work package, I will initially conduct multi-chamber multi-anvil experiments at 10 GPa and 2200C. Capsule materials will be the siderophile metal of interest, preloaded with a small amount of metal oxide to buffer the system. Silicate melt powders of different compositions will be loaded into the capsules. Previous experiments on hydrous melts have shown that pressure is sufficient to close the system when metal foils are used as lids, even in the presence of melt (Myhill et al., 2016). Samples will be heated, held at temperature for long enough to reach equilibrium (this should be <5 minutes, but timescales will be assessed during the experiments) and then quenched. Samples will be recovered and exposed, and then trace element concentrations in the melts will be measured using LA-ICP-MS. Activity coefficients will then be calculated (assuming a certain valence state) via the following expression:

MOn/2 = M + n/4 O2

Dependent on the magnitude of variations in activity coefficient for different elements, further experiments will be conducted to investigate the effects of varying P, T and oxygen fugacity.

**(Wood and Wade, 2013)**

*Figure XXXX: Activity coefficients derived*

**(WP3) Thermodynamic/thermoelastic models of the deep mantle and core of Mars.**

**Thermodynamic models are a vital requirement of calculating the density and seismic velocities within a planet as a function of pressure, temperature and composition. They can be used to calculate mineral compositions which are in equilibrium with each other, and also predict bulk densities and seismic velocities. Currently, published mineral models relevant to deep planetary interiors lack ferric iron end-members, which may be extremely important in terms of phase equilibria in the deep mantle (see WP1). In addition, thermodynamic models of core-forming materials are currently in their infancy; there is no model which accounts for the incorporation of sulfur, oxygen and silicon into liquid iron at high pressures. In this work package, I will create a model for majoritic garnets incorporating ferric iron, based on literature data and the results from WP1. I will add sulfur to the self-consistent thermodynamic model for light element incorporation into metallic melts that I have been building with Professors Dan Frost and Dave Rubie at the Bayerisches Geoinstitut, Germany. The addition of sulfur will allow us to take a potential core composition and predict densities and seismic properties, which can then be compared with those obtained from the InSight Mission.**

*The new experimental results from WP1 will allow much more accurate models of Mars' interior to be produced becuase ...... This will allow fully self-consistent interior models, which can be used to better interpret the insight data.*

Thermodynamic models of core liquids are still at a very preliminary stage. It has been noted that excess bulk moduli are likely to play a significant role in determining the properties of metallic solutions (Komabayashi, 2014), but so far there has been little attempt to create such a model. Working with Dan Frost and Dave Rubie, I have built a thermodynamic model for Si and O in metallic melts (Myhill et al., in prep), using modifications to existing solution models that enable excess bulk moduli to change in a physically reasonable manner as a function of pressure and temperature. This work package seeks to extend that model by adding sulfur, using existing experimental data (e.g. Buono and Walker, 2011; Tsuno et al., 2011).

Badro et al., 2013, Stevenson, 1989

*Figure XXXX: Modelled silicon and oxygen partitioning in metallic iron at 25 and 130 GPa, in comparison with independent (non-fitted) experimental data. One of the aims of this work package is to add sulfur to the model.*

Products from project:

* Improved garnet thermodynamic model enabling the calculation of chemical properties in Mars' deep mantle
* A preliminary Fe-Si-O-S metallic/sulfidic melt model, created using 1 bar, high pressure static, and shock data.
* Seismic velocities corresponding to the deep mantle and core of Mars, as a function of pressure, temperature and composition.

**(WP4) Geophysical modelling of Mars and an assessment of parameter trade-offs and uncertainties.**

**Creating forward models for Mars' interior provides an efficient way to investigate the effects of different variables on geophysical observables, such as seismic travel times or the moment of inertia. There have not currently been any attempts to systematically investigate the trade-offs between different variables. This is particularly true of Mars' thermal structure and composition, partly because of the unknowns addressed in WP1 and 3, and also partly because of choices of free variables and the richness of information contained in synthetic waveforms. In this work package, I will build interior models of Mars spanning the full range of plausible thermochemical structures, and analyse the trade-offs and uncertainties in parameters of interest in terms of InSight observables (e.g. P-S differential times, receiver functions, core properties, surface heat flow).**

Priors for our forward modelling will be the mass, moment of inertia and k2 Love number of Mars, an assumption of chemical equilibrium in the mantle and core and isentropic temperature gradient in the middle of the mantle and within the core. I shall use mineralogical models from the literature (e.g. Stixrude and Lithgow-Bertelloni, 2011), enhanced by the results from WP1,3.

The free parameters will include the Mg number and SiO2 content of the mantle, thickness of the crust, lithosphere and mantle, composition of the core, and thermal structure parameterised as mantle potential temperature, amount of internal heating and Rayleigh number (a measure of convective vigour). This parameterisation (which follows McKenzie et al., 2005) has the benefit of being physically meaningful, with parameters of geologic interest, whilst automatically including oft-ignored thermal features such as a lower boundary layer. Recently published thermal models include huge variability in thermal properties; two estimates of the thickness of the conductive lid/thermal boundary layer are 125/~200 km (Nimmo and Faul, 2013) and 400/~600 km (Khan and Connolly, 2008). Such variations change the moment of inertia significantly and will therefore trade-off against core properties. Seismic data from InSight should therefore provide important constraints on core properties, even if no core phases are observed.

I will use the forward models which fit the prior constraints (within uncertainties) to create synthetic waveforms (using TauP, SpecFem). I am currently collaborating with Stefanie Hempel (ISAE Toulouse) to set up the required workflow, taking advantages of new software functionality such as the ability to create synthetics for an oblate spheroid. From these, I will identify diagnostic waveform properties and parameter trade-offs. This study will enable rapid interrogation of data when it arrives from InSight.

*Figure XXXX: Example 1D seismic model of Mars, fitting the mass and moment of inertia of the planet and geochemical estimates of heat-producing elements (U, Th and K). Model includes thermal boundary layers at the top and bottom of the convecting mantle, and a mechanical boundary layer with experimentally-constrained temperature-dependent conductivity. Such models can be used to create synthetic seismograms of the Martian interior.*

*Figure XXXX: Core properties for a simplified set of Martian models*

*Figure XXXX: Some sort of trade-off figure? Example waveforms?*

**b) Management plan – Management of the project and resources, training and development opportunities**

I have previously held a two year Humboldt Fellowship in Germany, designing and running my own projects involving high pressure experiments. I am well-versed in multi-anvil techniques. I have written papers as a first author with co-authors from different countries.

The University of Bristol conducts annual staff reviews with a senior member of the research staff to ensure research goals are met. It has a comprehensive staff development program, running courses on project management, research leadership. The Faculty finance team provide support for resource management and purchasing.

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|  | 01-04/2018 | 05-08/2018 | 09-12/2018 | 01-04/2019 | 05-08/2019 | 09-12/2019 | 01-04/2020 | 05-08/2020 | 09-1/2020 |
| WP1 (Majorite) | E | A | W1 | W2 |  |  |  |  |  |
| WP2 (Partitioning) |  |  | E | E | A | W3 | A | W4 |  |
| WP3 (Modelling) |  | M | M/W5 |  |  | M | W6 |  |  |
| WP4 (Mars Structure) |  |  |  | A | A/W? | A/W? | A/W? | A/W? | A/W? |

E = Experiments; M = Model creation; A = Analysis of results; WX = Write up of paper X

? = Dependent on data acquisition

**c) Relationship to earlier or current work of the applicant/collaborating organisations, relevant work elsewhere**

I am currently working on InSight as a PDRA with Nick Teanby and James Wookey on a UKSA grant to study seismometer deployment, regolith properties, and shallow seismic events. On the InSight team I have set up collaborations on synthetic waveform generation with Dr Stefanie Hempel (ISAE Toulouse), which will feed in to WP3-5 of this project.

I have previous experience on passive seismic techniques, having worked on deep earthquakes for four years as a PhD student at the Bullard Laboratories, University of Cambridge. Following that, I spent three years conducting high pressure experiments at the Bayerisches Geoinstitut as a Humboldt Research Fellow and am well-versed in large and small-volume multi-anvil techniques up to 25 GPa. I have also developed thermodynamic models for high pressure mineral and melt phases in collaboration with Professors Dan Frost and Dave Rubie. I am also one of the developers of the BurnMan project, an open-source thermoelastic and thermodynamic toolkit, collaborating with Professor Timo Heister (U.S.A.) and Dr Sanne Cottaar (University of Cambridge).

The proposed research will compliment the existing work at Bristol and in the wider InSight team. There is currently no-one on the InSight team undertaking high pressure experiments or looking at the effects of sulfur and redox state on the questions targeted by the mission. This work will provide a real benefit to many others on the mission, feeding in to larger projects such as the Mars Structural Service, which is aiming to provide near-real-time updates to our best-guess model of Mars' interior.

**d) Justification of Resources Requested**

**Salaried Costs**

I will spend 100% of my time on the project, the salary is in line with standard UoB banding for a research fellow with 5 years of experience.

**Computing Costs (£9000)**

The main computing requirement is a desktop that is sufficiently high-specification to create synthetic waveforms from high resolution interior structure models using SpecFEM (£5000). Other costs include a laptop (£1000), data archival hardware (£1500) and other lab and computing consumables (£1000)

**Experimental Costs (£8640)**

Most multi-anvil experiments will be conducted at the University of Bristol, with some large volume/high pressure runs at the Bayerisches Geoinstitut, Germany. Costs per multianvil experiment (~£200 average over 36 experiments) take into account assembly costs (£50), cube breakage (~£200/cube), maintenance and machining, and analysis (LA-ICP-MS, majors via EPMA and ferric iron via Mössbauer spectroscopy). It is expected that there will be some heater failures due to LaCrO3 imperfections. For this reason, total costs are incremented by 20%.

**Travel costs**

* 2 team meetings per annum – during the two years of the mission, there will be quarterly team meetings, but as a relatively junior member of the team, I shall not be required to attend all meetings.
* 1 conference per annum – I intend to present results from this project at the LPSC (Texas), the AGU Fall Meeting (normally in San Francisco) and other academic meetings.
* 1 collaborative visit per annum – I shall be working with researchers in Germany, the States, and France.

2) Impact and outreach plan: one side, 11pt text (A4 paper, with minimum 2cm

margins)

3) CV

4) Publications list

5) Statement from the HoD

6) Two references (one from host institution, including advantages gained from hosting the fellowship)

7) Letter of support from UK instrument team member

**Objectives**

This proposal is to prepare for and analyse data from the SEIS experiment onboard NASA's InSight Lander, due to reach Mars in November 2018. The main objectives are:

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**Summary**

**Academic beneficiaries**

**Impact Summary**

Public Outreach:

Space travel and planetary formation are both extremely popular topics, and the work in this project provides an ideal opportunity to engage the public.

The work contained within this proposal will be used during Outreach events, such as those regularly conducted by @-Bristol. The PI has already conducted successful seismological outreach with @-Bristol.

The School of Earth Sciences works regularly with this museum. Bristol is also part of a recently funded UKSA public engagement project 'Marsquake Monitor: measuring the pulse of the planet', led by Paul Denton (British Geological Survey), which aims to provide school-age children with the opportunity to perform seismic experiments and analyse real mission data. The work from this project would provide excellent material to provide children with easily understandable and testable hypotheses.

Education:

The PI has recently been involved with the Global Summer School, hosted by Imperial College London, which aims to provide engineering-track A-level students with insights into real world applications. The school includes two focused days on Mars missions, and is already starting to incorporate InSight into the teaching schedule. The proposed work would provide a perfect scientific “big-picture” for teaching purposes.

The development of thermodynamic and thermoelastic models will be conducted with BurnMan, an easy-to-use, modular thermoelastic toolkit (Cottaar et al., 2013). One of the planned additions for BurnMan is a graphical planet builder, where a user can input a bulk composition and planetary structure and visualise the effects of structure and planetary evolution on observables such as mass, moment of inertia and seismic profiles. Three months of project time are devoted to implementing this functionality and an associated GUI, for use as an educational web-tool. One of the other developers of BurnMan (I. Rose) has developed a web applet to teach school children about mantle convection and global seismology (http://ian-r-rose.github.io/interactive\_earth/thermal\_hires.html), and the two projects could easily be combined to demonstrate the propagation of seismic waves on Mars.

NOTES:

On Earth, the state of disequilibrium between the core and the mantle are further constrained by a large number of high pressure experiments on Earth-like compositions, and a vast quantity of seismic and other geophysical data. To link the experimental and seismological data, detailed thermodynamic/thermoelastic models are required. Such models are currently in their infancy (Komabayashi, 2014). The PI is currently extending and improving such models with flexible equations of state that can be used to match multi-anvil, diamond-anvil, shock and ab-initio experiments, both for silicate melts (de Koker et al.) and metallic melts (Anderson and Ahrens, 1994). These models are further informed by melting curves, 1 bar data and equilibria experiments (Myhill et al., in prep.). The author has also developed modifications to existing solution models to allow excess bulk moduli (Myhill, in review), thermal expansion and heat capacity data to be modelled; additions which are vital for high pressure phase equilibria and seismic velocities (e.g. Williams et al., 2015).

Gaetani and Grove (1996) Important constraints on core formation in Mars are provided by our experimental determination of the partitioning of Cu between silicate and sulfide melts. When combined with existing estimates for siderophile element abundances in the Martian mantle and a mass balance constraint from Fe, the experiments allow a determination of the mass of the Martian core (∼17 to 22 wt% of the planet) and its S content (∼0.4 wt%). These modeling results indicate that Mars is depleted in S, and that its core is solid.

MSE abundances on Earth suggest moderate pressure equilibrium (25-60 GPa, 2200-4000 K, mostly based on Ni,Co), see summary in Rubie et al

HSE abundances on Earth and Mars are similar (Warren et al., 1999) and in chondritic abundances, but pressures and temperatures of core formation were presumably quite different; support for late veneer (e.g. Righter, 2005).

Wade and Wood (2005) suggested continuous core accretion based on MSE, require low fO2 early in Earth history. Problem is that tantalum is highly siderophile under reducing conditions, but is present in chondritic abundance in the Earth (Mann et al., 2006).

Jones and Drake (1986) – inefficient core segregation (trapped metal fraction).

Rubie et al. suggest Mars more reduced because no Fe3+-rich pv layer.

Hustoft and Kohlstedt (2006) – deformation enhanced percolation

Wood et al., 2006 suggest from chondritic model, using elements of similar volatilities to adjust for loss to space:

85% Fe,

5% Ni,

0.9% Cr,

0.25% Co,

~1.9 wt% S (1.5-2.0 from McDonough, 2003),

0.2 P

0.2 C

0.1 H

6–7 Si, O (proportions controversial)

Rudge et al., 2010 suggest >=36% of Earth's core formed in eqm with mantle

Tuff et al., 2013 – early oxidation of a sulphur rich mantle.

Boujibar et al., 2016 – perovskite-melt more complex in Fe3+ than previously thought.

Wood, 2008 – Earth requires oxidation during growth

Georg and Shahar, 2015 – Earth requires reduction during growth

Jana and Walker (1997) – Fe ↔ FeS effect on MSEs, HSEs, lithophiles, chalcophiles.

Boujibar et al (2014) – FeS on quench … reflects magma ocean solubility?

Elkins-Tanton et al., 2003 – Mantle overturn – alumina segregation into the deep Mars mantle.

Tait and Jaupart (1992) – Mush thin when reacts

Dynamo driven by early S-rich core followed by late, more Fe-rich core material?

From WP2

It has been suggested that the reduced, iron rich mantle of Mars is a consequence of low magma ocean temperatures in Mars (Rubie et al., 2004).

Righter and Chabot, 2011

Q. How to design sulfide melt system?

add nickel and cobalt? “free” partitioning experiments

Bonus – dihedral angle study. (Terasaki et al.)

The concentrations of the moderately and highly siderophile elements in the SNC meteorites have been used to imply the rapid formation of a core by segregation from a deep magma ocean. Published estimates of pressures and temperatures vary widely, even for Earth (Rubie et al., 2007). Part of the problem may arise from modelling core formation as a single-stage process, despite accretion occuring via oligarchic growth.

Finally, isotopic heterogeneity in Nd, Hf, Os recorded by different groups of the SNC meteorites indicates that Mars' mantle preserves distinct primordial reservoirs generated by early silicate differentiation processes (Lee and Halliday, 1997; Foley et al., 2005; Borg and Draper, 2003; Brandon et al., 2012; Mezger et al., 2013).

1. **Remote geophysical.** Mars' mass, radius and moment of inertia tell us that Mars has a dense metallic core surrounded by a silicate mantle. Tidal dissipation (specifically, the k2 Love number) tells us that at least the outer part of the core is likely to be fluid. If the mantle has no interconnected melt, the data indicates that the core has a radius of 1520-1840 km (Yoder et al., 2003). For a core of this size to match the moment of inertia observations, it must have a density less than that of solid iron, but the uncertainties in core radius and thermochemical structure in the mantle and crust lead to very large uncertainties in composition.
2. **Geochemical.** The compositions of rocks observed by the Mars rovers, and the Shergottite-Nakhlite-Chassignite (SNC) meteorites imply that, compared with Earth, Mars is rich in iron (Mg# ~ 75; Wanke and Dreibus, 1994) and sulfur (2000 ppm; Tuff et al., 2013), but has a low oxygen fugacity and low water contents. It has therefore been suggested that the core is rich in sulfur. Nevertheless, these interpretations rely on the sampled surface rocks being representative of the deep interior. Even if they are, the range of proposed sulfur contents is huge: Gaetani and Grove (1997) suggest ∼0.4 wt % S in the core, while Wanke and Dreibus (1994) suggest 14 wt %. On the basis of iron isotope fractionation, Shahar et al. (2015) suggest 0-8 wt % S, while geophysical modelling by Khan and Connolly (2008) suggests >20 wt %, and possibly as high as 36 wt % (pure FeS). Such different values imply very different formation and cooling histories of Mars.

Mailis

Hernlund/Labrosse – temperatures can be much higher than the liquidus for equilibriation (Abstract AGU, 2014)

In order to constrain the interior structure and evolution of Mars from raw InSight data, it is vitally important to have good thermodynamic models to calculate density and seismic wave velocities from pressure, temperature and composition. These can be used to build forward models of the Martian interior, using appropriate parameterisations for thermochemical structure. Finally, these models can be used to create synthetic waveforms which can be compared with the data returned from InSight. Although this workflow is well-structured and straightforward to implement, our current understanding of the inputs is less-than-ideal. The proposed project proposal contains work packages designed to address the following major gaps in our understanding:

* The mantle models neglect interaction between silicates and metallic/sulfidic species which are likely to be important on an iron- and sulfur-rich planet such as Mars (WP1,3).
* The interactions between these species during Mars' formation must have dictated the present day composition of the core, but the data necessary to perform a joint inversion does not yet exist (WP2).
* Simple core formulations fail to incorporate the complex relationships between core composition and physical properties such as density, isentropic gradient and bulk modulus, which are required to model the density and Vp structure of the core (WP3).
* Key parameters which are currently overlooked in modelling Mars' thermal structure are the Rayleigh number of the mantle and proportion of internal heating, which affect the thermal boundary layers at both the top and bottom of the mantle, and therefore the moment of inertia and seismic velocities (WP4).
* All of these gaps in our scientific understanding should be addressed before attempting to create a synthesis of Mars' formation, evolution and present-day state (WP5).