

# First-principles investigation of equilibrium iron isotope fractionation in Fe<sub>1-x</sub>S<sub>x</sub> alloys at Earth's core formation conditions

CARLOS PINILLA<sup>1</sup>, ALDEMAR DE MOYA<sup>1</sup>, GUILLAUME MORARD<sup>2,3</sup>, SÉGOLÈNE RABIN<sup>4</sup>, MATHIEU ROSKOSZ<sup>5</sup> AND MARC BLANCHARD<sup>6</sup>

<sup>1</sup>Universidad del Norte

<sup>2</sup>Université Grenoble Alpes-CNRS-IRD-IFSTTAR-ISTerre

<sup>3</sup>Sorbonne Universités-IMPIC-UMR-CNRS 7590 IRD

<sup>4</sup>Géosciences Environnement Toulouse

<sup>5</sup>Sorbonne Universités-IMPIC-MNHN-UMR-CNRS

<sup>6</sup>Géosciences Environnement Toulouse - CNRS - Univ Toulouse III - IRD - CNES - OMP

Presenting Author: [ccpinilla@uninorte.edu.co](mailto:ccpinilla@uninorte.edu.co)

Iron is one of the most abundant non-volatile elements in the solar system. As a major component of planetary metallic alloys, its immiscibility with silicates plays a major role in planetary formation and differentiation. In particular, recent attention has been paid to <sup>56</sup>Fe/<sup>54</sup>Fe equilibrium isotope fractionation at conditions relevant to Earth's core formation and the influence that light elements (O, H, C, Ni, Si and S) have had in this process. Most of these experimental studies relied on the measurement of Fe isotope fractionation from quenched phases of silicate melts and molten iron alloys. The experimental works are extremely challenging, and may suffer different drawbacks. To overcome this, we use *ab-initio* computational methods to perform a systematic study of the <sup>56</sup>Fe/<sup>54</sup>Fe equilibrium isotope fractionation in molten and solid Fe<sub>1-x</sub>S<sub>x</sub> alloys at conditions of the core formation (60 GPa, 3000 K). We show for the first time, that equilibrium isotope fractionation factors from solid systems can be used as proxies for molten systems. Additionally, we discuss the effect of sulphur concentration on the equilibrium Fe isotope fractionation and show that although there are some structural changes due to atom substitutions, the wide range of studied concentrations produces fractionation factors that are constant within ~ 0.01‰. Finally, we discuss the implications of our results for the interpretation of recent experiments and the understanding of core crystallization processes.