

Large-scale atmosphere dissolution in magma oceans in exoplanets

SUPPLEMENTARY INFORMATION

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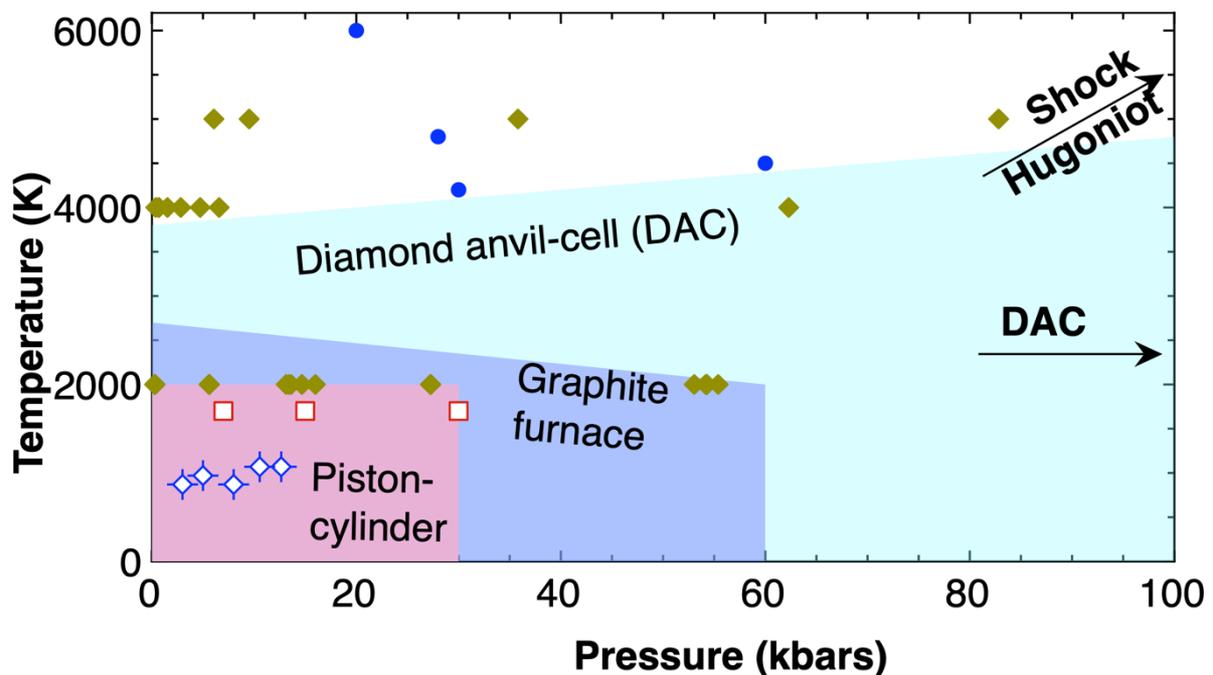


Figure S1. Typical limits of the different experimental techniques, their relation with the estimated conditions occurring at the atmosphere – rocky core interface in various sub-Neptunes (blue solid circles)¹ and the conditions reached in our atomistic molecular dynamics simulations (solid rhombi). The experimental limits are intrinsic to the materials used, like the melting line of diamond^{2,3} (light blue rectangle) or graphite⁴ (dark blue rectangle), or the inherent mechanical failures of steel components of the piston-cylinder presses⁵ (fuchsia rectangle). Empty squares⁶ and empty diamonds⁷ give the conditions attained in the two sets of piston-cylinder experiments on hydrogen-melt solubility.

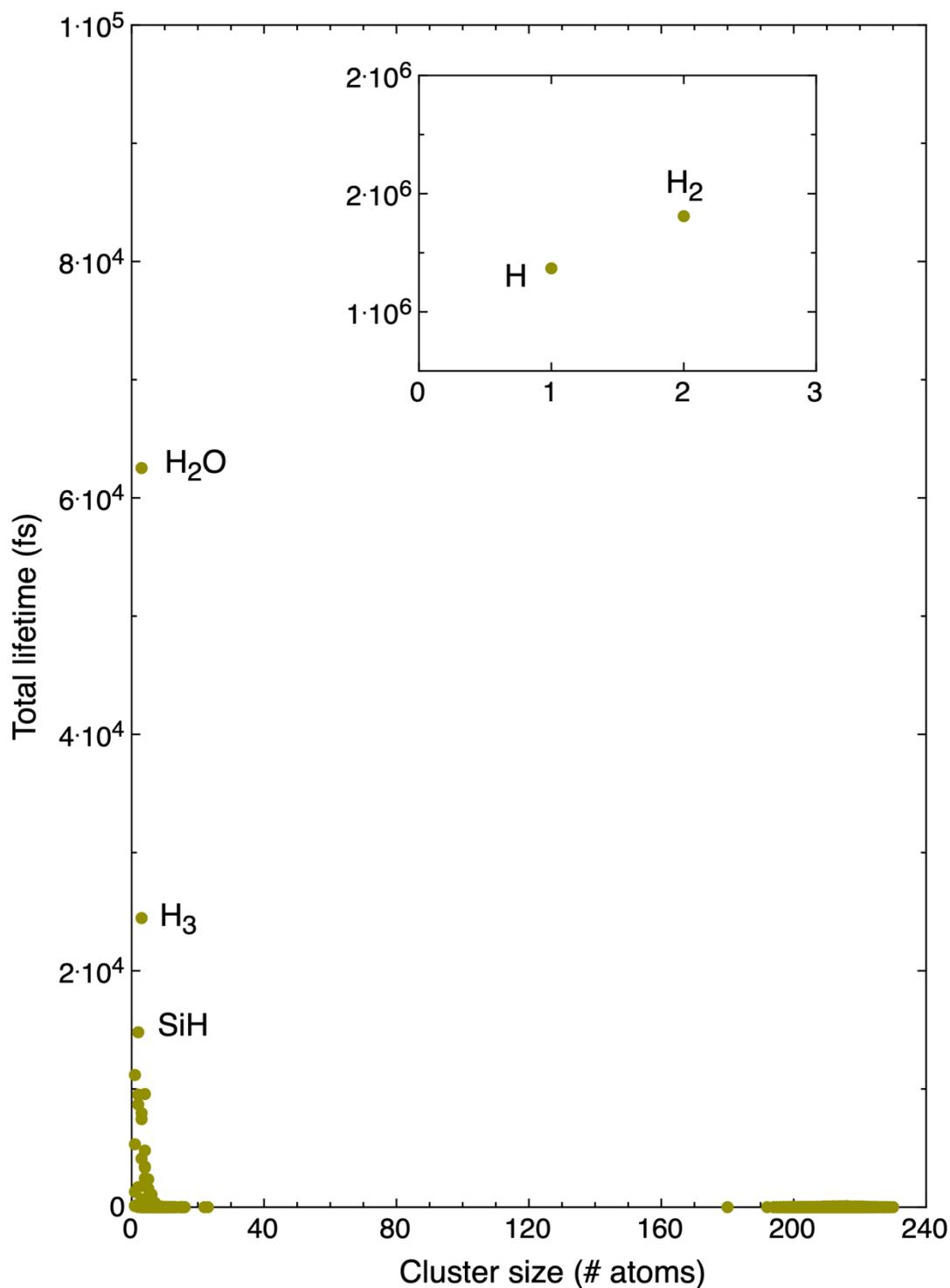


Figure S2. Typical bimodal distribution of the sizes of the atomic clusters encountered in the simulations. The large clusters, to the right of the diagram represents the polymerized silicate liquid. The small clusters, to the left of the diagram represented the non-polymerized gas phase. Note that the atomic and the molecular hydrogen dominate by two orders of magnitude the statistics of the population – but at all conditions this hydrogen is unbounded, representing the atmosphere that reacts with the underlying silicate.

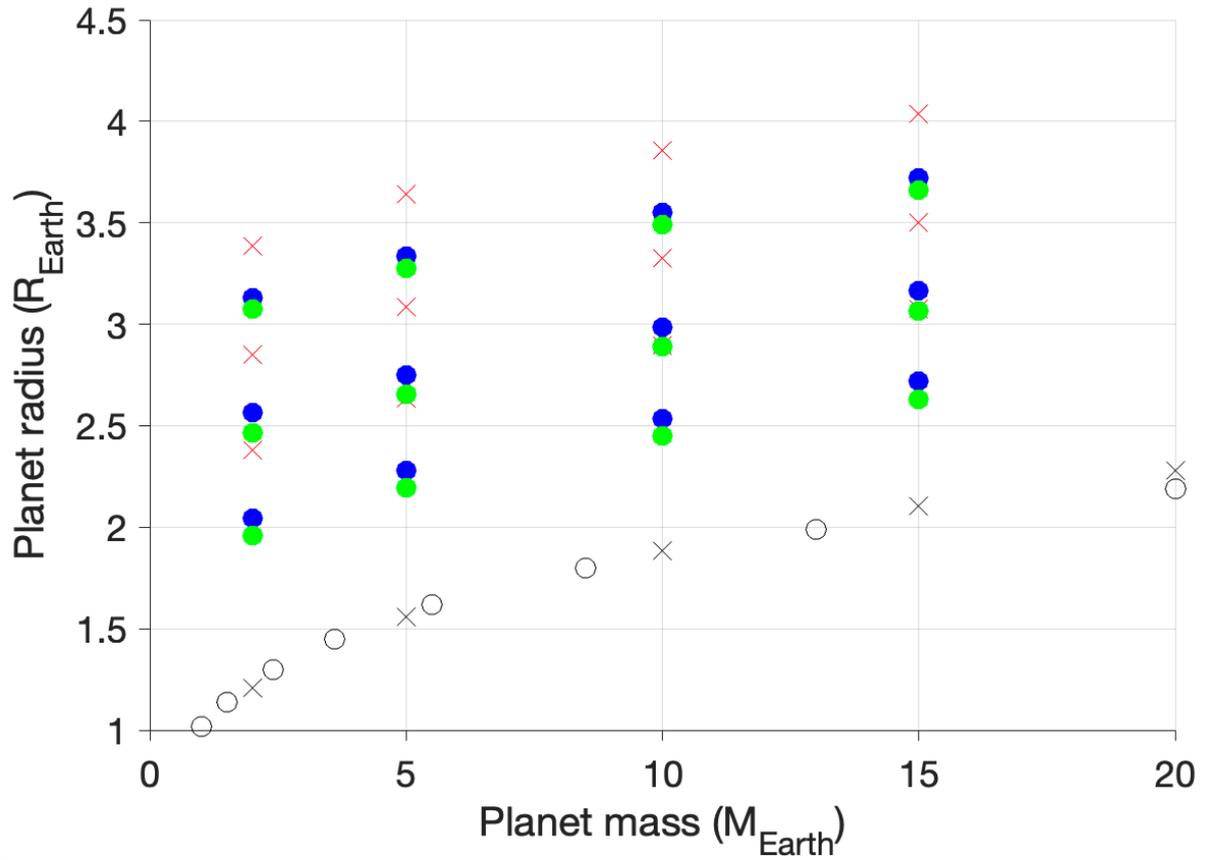


Figure S3. Estimated planetary mass-radius relations combining molecular dynamics (MD)-derived solubilities with MESA structure models. Green dots show MESA radii assuming no dissolution, for envelope mass fractions of 2, 5, and 10 wt%. Blue dots include approximate corrections for hydrogen dissolution into the core and associated core expansion ("puff-up"). Red crosses indicate extreme puff-up without dissolution, for reference. Black symbols correspond to the bare-rock case.

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