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# Pressure-driven evolution of phosphorus speciation in lower mantle melts: Insights from ab initio molecular dynamics

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Phosphorus (P) is a critical element influencing the origin and evolution of life, and its availability is intricately linked to global tectonics and biogeochemical cycles. While it is well established that P primarily exists in Earth's crust as phosphate minerals (except for phosphite in early Earth's sediments), its behavior under extreme conditions in Earth's deep interior remains inadequately understood, particularly regarding its enhanced siderophilicity during core formation. This study employs ab initio molecular dynamics simulations to investigate the structural evolution of P in pyrolitic melts under lower mantle conditions, focusing on its coordination environment and interactions with iron (Fe). Our findings reveal that as pressure increases from 0 GPa to 135 GPa, phosphorus undergoes a gradual densification, transitioning from predominantly tetrahedral coordination to approaching octahedral coordination at the core-mantle boundary. Notably, although P coordination increases steadily with pressure, the transition occurs more slowly compared to silicon and aluminum, likely due to the π-component of the P–O bonds, which resists structural changes. Importantly, the predominance of high-spin Fe in lower mantle melts indicates that using non-spin-polarized approximations for Fe can lead to erroneous representations of P-Fe interactions and introduce non-existent phosphorus speciation. This has significant implications for understanding the siderophile behavior of P under high pressure, as the interactions between Fe and P may influence the stability and speciation of P in these environments. Therefore, a careful reevaluation of the siderophile nature of P is warranted, particularly in systems that accurately account for the spin state of Fe.