Abstract Submitted
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Symmetry breaking in a dense liquid: Why sodium melts at room temperature.[1] JEAN-YVES RATY, University of Liège, Belgium, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Dalhousie University, Canada — The melting curve of sodium measured in [1] exhibits unusual features under pressure : the melting temperature, Tm, reaches a maximum around 30 GPa followed by a sharp decline from 1000 K to 300 K in the pressure range from 30 to 120 GPa. In this study, the structural and electronic properties of molten sodium are studied using first principles theory. With increasing pressure, liquid sodium initially evolves by assuming a more compact local structure, which accounts for the maximum of Tm at 30 GPas. However, at pressure around 65 gigapascals a transition to a lower coordinated structure takes place, driven by the opening of a pseudogap at the Fermi level. Remarkably, the broken symmetry liquid phase emerges at rather elevated temperatures and above the stability region of a closed packed free electron-like metal. The theory explains the measured drop of the sodium melting temperature, down to 300 kelvin at 105 GPas. [1] Gregoryantz et al., Phys. Rev. Lett. 94, 185502 (2005).

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