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**Properties of molten sodium under pressure from first principles theory.**[1] JEAN-YVES RATY, University of Liege, Belgium, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Dalhousie University, Canada — Recent measurements of the melting curve of sodium [1] have found a sharp decline in the melting temperatures from 1000 to 300 K in the pressure range from 30 to 120 GPa. In this study, we investigate the stability and structural properties of solid and liquid sodium at high pressure and temperature using first principles molecular dynamics. The experimental melting curve is reproduced from 0 to 120 GPa. The local structure of the liquid is found to be strongly correlated to the multiple finite temperature crystalline phases of sodium. Based on a quantitative analysis of the structural and electronic properties of the solid and liquid phases, we propose an explanation for the unusual melting curve and a new perspective on the phase diagram of sodium. [1] Gregoryantz et al., Phys. Rev. Lett. 94, 185502 (2005).

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