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Complexity in 'simple' metals[1] BRUNO ROUSSEAU, NEIL W. ASHCROFT, Cornell University — In electronic and structural terms, the light alkalis have long been regarded as 'simple systems', at least under ordinary conditions. However, when compressed they exhibit unforeseen complexity; the melting curve of sodium, for example, has a striking maximum, falling to near room temperature melting where a complex structure (CI16) is found, this being in the cubic class but with 16 atoms per unit cell [1,2]. The light alkalis have been extensively studied using ab initio methods with standard assumptions of transferability made for the key pseudopotential input information, largely atomic based. Lacking still, however, is a somewhat more intuitive and physical understanding of the developments in electronic structure with progressive increase in density. In the present work, the problem is treated with non-linear response theory and non-overlapping pseudopotentials, and the structural complexity traced to effective ion-ion interactions with features that both at short range and long display competing state dependence.

[1] Gregoryanz et al., Phys. Rev. Lett. 94, 185502 (2005)
[2] McMahon et al., Chem. Soc. Rev. 35, 943 (2006)

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