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Ab initio studies of electronic and structural transitions in low-Z liquids under extreme conditions[1]

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The liquids of group I elements (H, Li, Na, and K) are studied using first principles theory. It will be shown that they undergo electronic and structural transitions analogous to that observed in their solids, but commencing at much lower pressure in the presence of disorder. These changes result in exotic melting behavior and in molten phases with unusual properties. The theoretical predictions will be compared with experimental data and ways for further experimental verification of the theoretical results will be suggested.

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