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Superconductivity of Li, Al and K under pressure GIANNI PROFETA, Univ. di L'Aquila (Italy) — C Franchini[§], N. N. Lathiotakis[†], A. Floris[†§], A. Sanna[§], M. A. L. Marques[†], M. Lüders[‡], S. Massidda[§], E. K. U. Gross[†], A. Continenza[*].

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Extreme pressure strongly affects the superconducting properties of "simple" metals, like Li, K and Al. Using the new ab-initio method of density functional theory of the superconducting state, we report investigations on the superconducting properties of dense Li, K and Al. Our results show an unprecedented agreement with experiments, assess the predictive power of the method over a wide range of densities and electron-phonon couplings, and provide predictions for K, where no experiments exist so far. For fcc K we predict a superconducting phase transition at 18 GPa, with a maximum critical temperature of about 2 K at 23 GPa, the pressure where the crossover between the fcc and the K III structure experimentally occurs. We studied the effect of pressure on the electronic and vibrational properties of alkali, showing a progressive phonon softening near the K point of the Brillouin zone and a concomitant enhancement of the electron-phonon coupling constant λ.

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