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Analytical Expression for a Pseudo-Potential in Alkali Metals

GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — In previous works [1-3] using a local first principles pseudo-potential, have been calculated interionic potential and thereafter different properties have been obtained from simple metals as phonon dispersion curves, phonon spectra, specific heats properly. The pseudo-potential is constructed from the electron density, which is previously calculated by the density functional theory. All this process is carried out numerically. The pseudo-potential has a similar behavior in the alkali metals and then we propose an analytical expression for it, which depends on the parameter rs, the atomic number and two additional parameters. This analytical pseudo-potential is used to calculated phonon dispersion curves, which are in good agreement with existing experimental reports, it is expected that the other properties calculated based on this pseudo-pontencial match with the experimental results.

- [1] Manninen M., et al, Phys.Rev. B 24 (1981) 7057
- [2] Ruiz, G., Physics Letters A 336 (2005) 210
- [3] Magaña, L.F. and Vázquez, G.J., Phys.Rev.B 36 (1987) 4700

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