

# On the origin of bonding in metals: sodium and chromium as case studies

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## Abstract

The bonding in metals is analysed within the framework of the PATMOS (Perturbed AToms in MOlecules and Solids) model. The binding energy per atom is written as a sum of a distortion energy of the atom and the partitioned interaction energy comprising Coulombic, exchange and correlation terms. On the basis of calculations on one-dimensional arrays of sodium and chromium atoms, the following conjecture is suggested. Metals are made of weakly interacting atoms, i.e. perturbed atoms. A proper description of bonding requires an unrestricted Hartree-Fock wave function as the basic approximation. Metals and molecules have in common the predominance of the Coulombic interatomic interaction energy. Electron correlation is of paramount importance.

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patmos\_metal\_bond.pdf available at <https://aurea.com/users/300490/articles/430173-on-the-origin-of-bonding-in-metals-sodium-and-chromium-as-case-studies>

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