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# Theoretical study of linear monoatomic nanowires, dimer and bulk of Cu, Ag, Au, Ni, Pd and Pt

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**Abstract**

The binding and electronic properties of monoatomic nanowires, dimers and bulk structures of Cu, Ag, Au and Ni, Pd, Pt have been studied by the projector augmented-wave method (PAW) within the density functional theory (DFT) using the local density approximation (LDA) as well as generalized gradient approximation (GGA) in both Perdew–Wang (PW91) and Perdew–Burke–Ernzerhof (PBE) parameterizations. Our results show that the formation of atomic chains is not equally plausible for all the studied elements. In agreement with experimental observations Pt and Au stand out as most likely elements to form monoatomic wires. Changes in the electronic structure and magnetic properties of metal chains at stretching are analyzed.


*Keywords:* Chain; Dimer; Bulk structures; Electronic and magnetic properties; DFT; Nanowires

## 1. Introduction

A proper understanding of the electronic properties of nanosized junctions is crucial for many domains of modern nanotechnology. Metal nanowires have recently attracted a great deal of attention due to their unusual properties and relative simplicity of fabrication. Most studied systems both experimentally [1–7] and theoretically [8–16] are free standing gold nanowires, which exhibit a quantized conductance at stretching and have peculiar structural properties. Unsupported and supported wires of Cu, Pd, Pt, Ag and Au have also been studied theoretically by means of *ab initio* and molecular dynamics methods [14,17–22]. The influence of relativistic effects on the properties of Pd and Ag wires is analyzed in Ref. [23] and it is shown that fully relativistic and scalar relativistic calculations give very similar results. Comparison of binding energies per bond in bulk and chain structures of noble metals allowed Bahn et al., to conclude that Au and Pt are more likely to form atomic chains than other noble metals [14].

Magnetic properties of metal chains have also attracted considerable attention [19,23–32]. In particular, it has been suggested that a magnetic ordering in Pd chains determines the conduction properties of the system [26]. Studies have shown that Ag wires are non-magnetic at equilibrium bond length in contrast to Pd chains exhibiting the magnetic moment of 0.7 $\mu_B$/atom at equilibrium interatomic separations [23]. The dependence of the magnetic moment on interatomic distance and wire structure has been studied in detail for Pd chains [24]. Short monoatomic Pd wires suspended between two Pd leads appear to have a moment of 0.3 $\mu_B$ whereas the coaxial nanowire is predicted to be non-magnetic [24]. Recently the density functional calculations employing the self-interaction corrected (SIC) LDA-functional have shown that the values of the magnetic moments for Pd wire are ~0.45 $\mu_B$ and 0.69 $\mu_B$ at equilibrium and break separations, respectively [25]. It is interesting to compare these results with magnetic moment of the Pd dimer which from *ab initio* pseudopotential calculations

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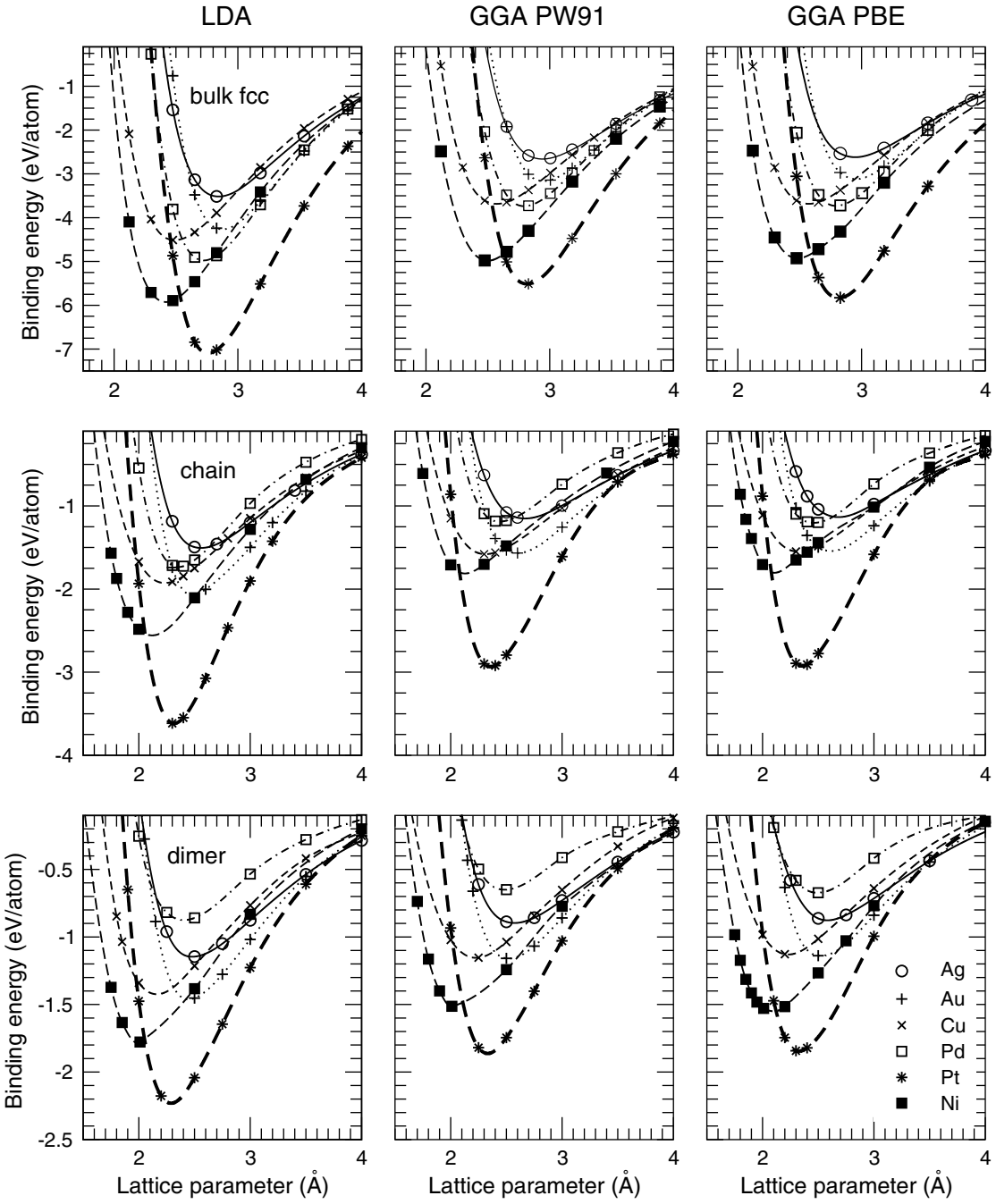


Fig. 1. Binding energy curves for fcc bulk, linear chain, and dimer structures of Cu, Ag, Au, Ni, Pd, Pt calculated within the LDA, GGA–PW91 and GGA–PBE approximations.

was found to be 1 $\mu_B$ per Pd atom [28–30]. The same result was obtained using a semi-empirical tight-binding method and SIESTA code based on the linear combination of pseudoatomic orbitals [31]. At the same time, a tight-binding model within the Hartree–Fock approximation resulted in a non-magnetic solution for Pd dimer [32]. Fully relativistic *ab initio* calculations done for Pt wires indicate that magnetic moment for Pt monowire is about 0.6 $\mu_B$ at the equilibrium bond length of 2.48 Å [20]. A review of electronic, magnetic, and structural properties of clusters including mono- and diatomic chains for metals in groups 10 and 11 is given in Refs. [30,33–35].

Here, we present the results of a systematic *ab initio* study of the binding energies, equilibrium lattice parameters, break forces and magnetic properties of the linear infinite chains of Cu, Ag, and Au as well as Ni, Pd and Pt. We analyze the dependence of these properties on the degree of wire stretching and compare them to those of dimer and bulk structures of corresponding materials.