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Theoretical Method for Full Ab-Initio Calculation of Rhenium Carbide Compound

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Abstract : First principles calculations are carried out to investigate the structural, electronic, and elastic properties of the utraincompressible materials, namely, noble metal carbide of Rhenium carbide (ReC) in four phases, the rocksalt (NaCl-B1), zinc blende (ZB-B2), the tungsten carbide(Bh) (WC), and the nickel arsenide (NiAs-B8).The ground state properties such as the equilibrium lattice constant, elastic constants, the bulk modulus its pressure derivate, and the hardness of ReC in these phases are systematically predicted by calculations from first–principles. The corresponding calculated bulk modulus is comparable with that of diamond, especially for the B8 –type rhenium carbide (ReC), the incompressibility along the c axis is demonstrated to exceed the linear incompressibility of diamond. Our calculations confirm in the nickel arsenide (B8) structure the ReC is found to be stable with a large bulk modulus B=440 GPa and the tungsten carbide (WC) structure becomes the most more favourable with to respect B3 and B1 structures, which ReC- WC is meta-stable. Furthermore, the highest bulk modulus values in the zinc blende (B3), rock salt (B1), tungsten carbide (WC), and the nickel arsenide (B8) structures (294GPa, 401GPa, 415GPa and 447 GPa, respectively) indicates that ReC is a hard material, and is superhard compound H(B8)= 36 GPa compared with the H(diamond)=96 GPa and H(c BN)=63.10 GPa.

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