Ab initio study of structural, mechanical and electronic properties of 3d transitional metal carbide in cubic rocksalt (rs) , zincblende (zb) , and cesium chloride (cc) structures by using LDA and GGA Approximation

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I. SUPPLEMENTARY INFORMATION

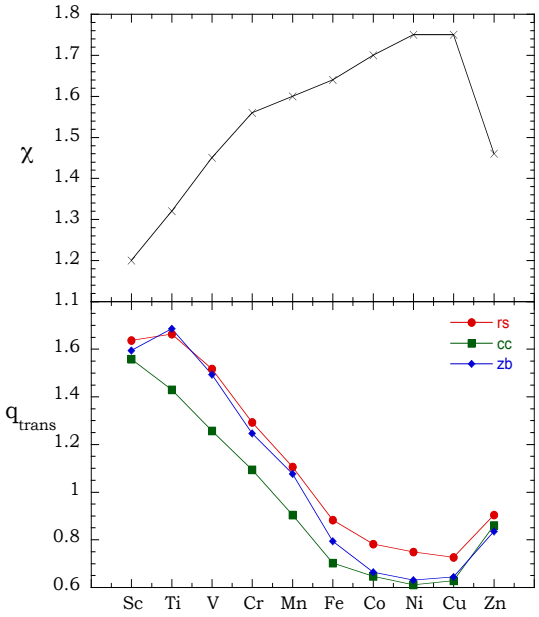

FIG. S1: Electronegativity (χ) from literature [1] of the transition metals and Bader charger transfer from metal atoms to carbon atom (q_{trans}) obtained from DFT calculation using GGA approximation.

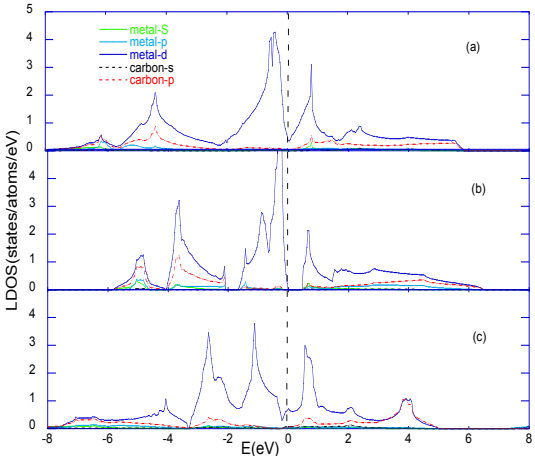

FIG. S2: Local density of states (LDOS) of FeC in rocksalt (a), zincblende (b), and cesium chloride (c). Fermi energy is set to zero in each panel.

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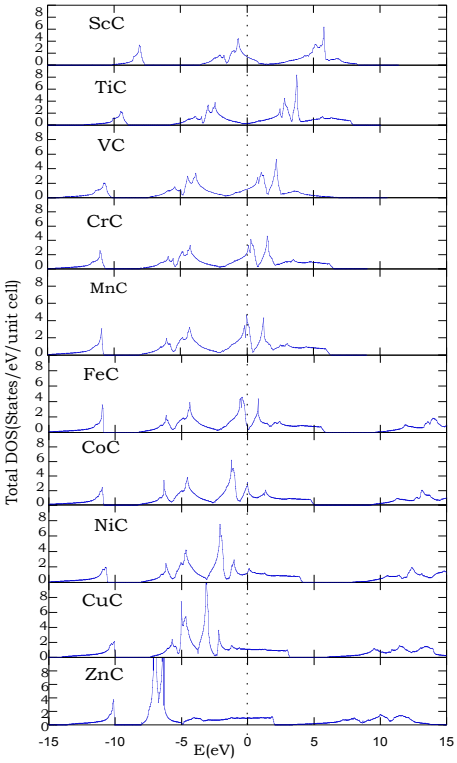

FIG. S3: Total density of states (TDOS) per formula unit of the 3d transitional metal carbides in rocksalt (rs) structure. Fermi energy is set to zero in each panel.

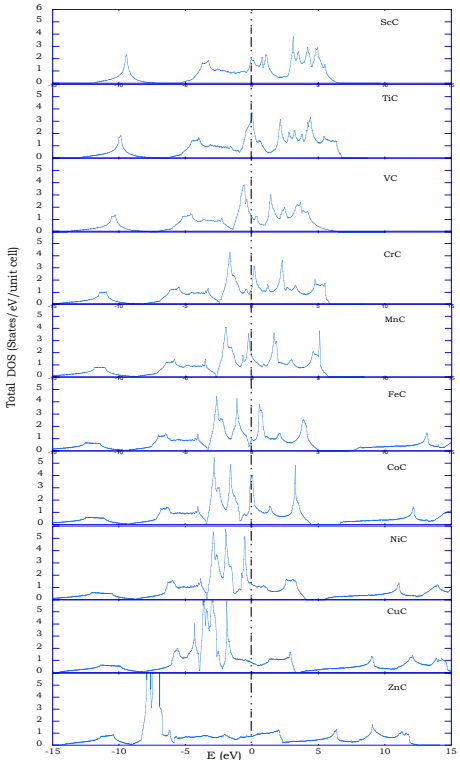

FIG. S4: Total density of states (TDOS) per formula unit of the 3d transitional metal carbides in cesium chloride (cc) structure. Fermi energy is set to zero in each panel

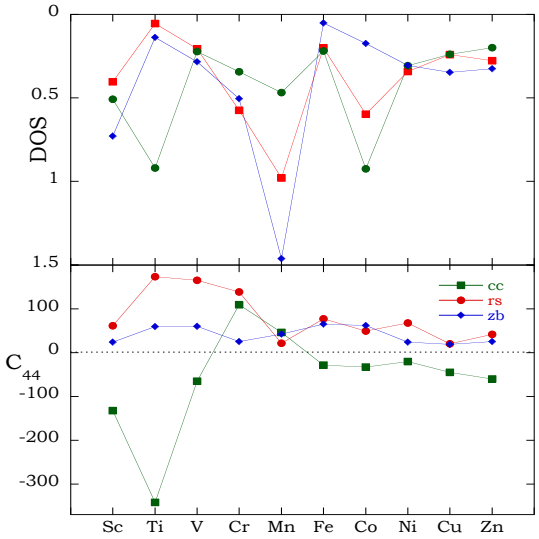

FIG. S5: The number of electronic states per formula unit around E_F integrated from -0.15 eV to 0.15 eV and elastic constant C_{44} of the carbides versus their corresponding 3d transitional metals. The y-axis in the upper panel is shown inverted.

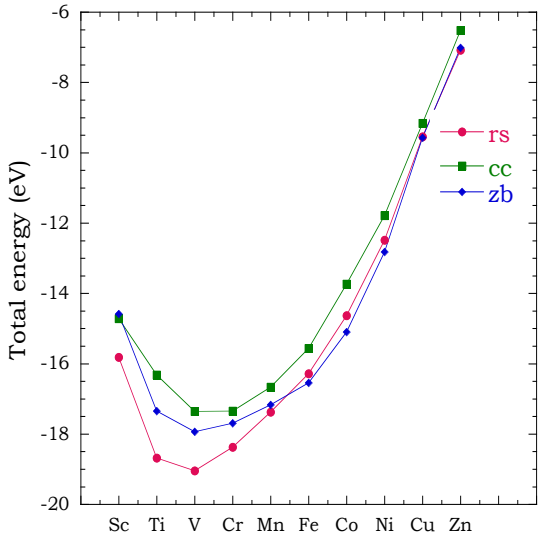

FIG. S7: total energy of 3d transitional metal carbides in zincblende (zb), rocksalt (rs), and cesium chloride (cc) structures..

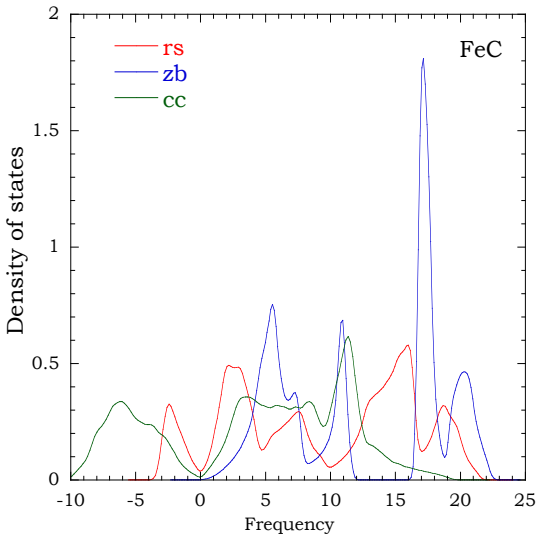

FIG. S6: Phonon density of states (DOS) of FeC.

[1] A.L. Allred, E.G. Rochow, A scale of electronegativity based on electrostatic force, J. Lnorg. Nucl. Chem. 5 (1958) 264?268, http://dx.doi.org/10.1016/0022-1902(58)80003-2.