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Unconventional superconductivity in 3*d* rocksalt transition metal carbides

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Supplementary Material of Journal of Materials Chemistry C 7, 12619 (2019)

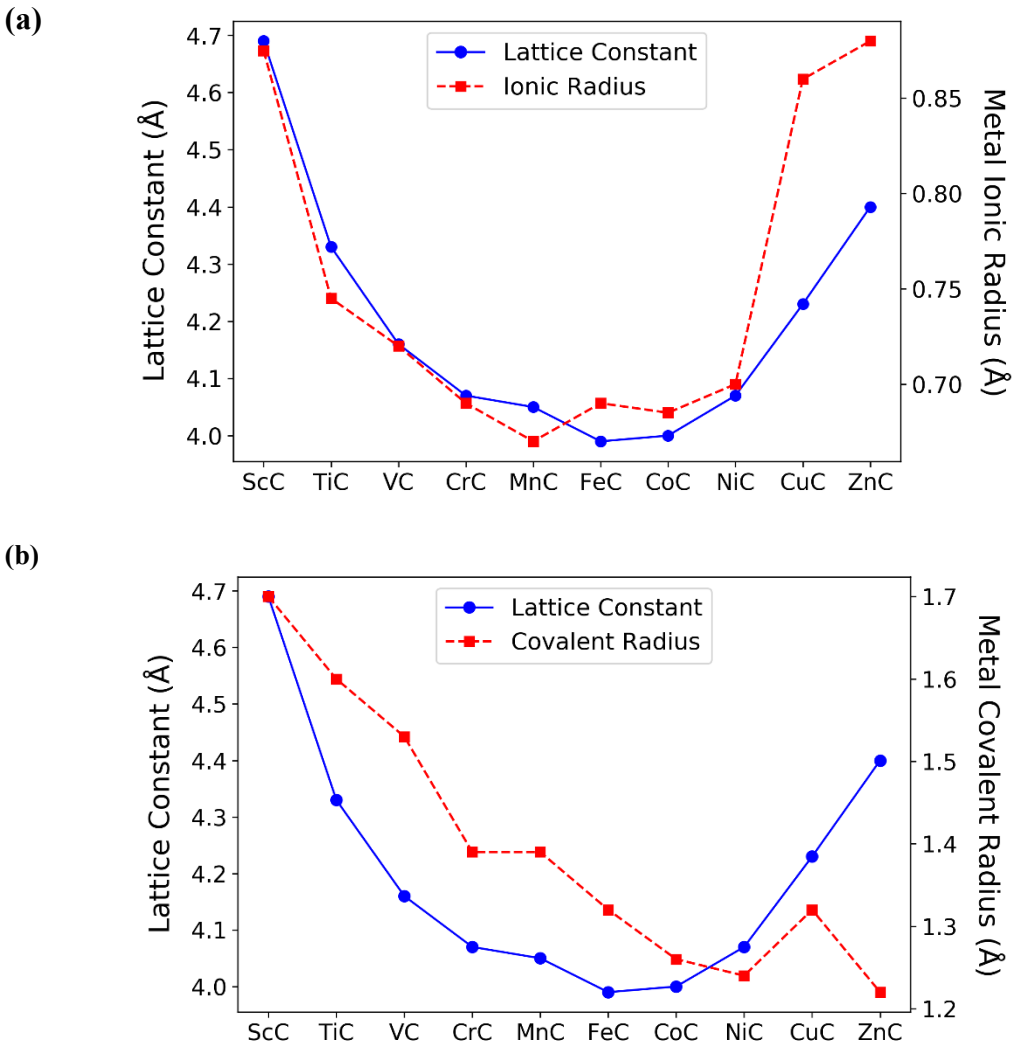


Figure S1: Correlations between calculated lattice constants and respective (a) ionic and (b) covalent radii of the transition metals for each compound. Values for ionic and covalent radii are taken from the literature [1].

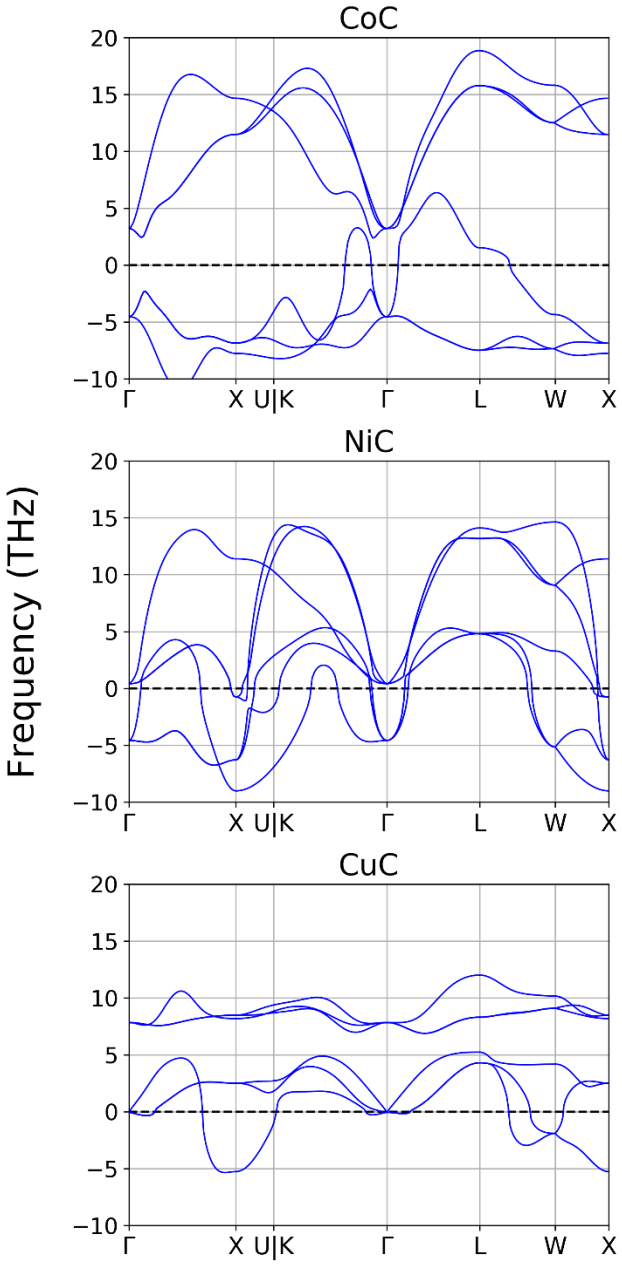


Figure S2: Phonon dispersion curves, calculated within the framework of the harmonic approximation, of the rocksalt 3*d* TMCs which are found to be dynamically unstable at all reasonable temperatures and pressures. Positive values are real, whereas negative values corresponding to imaginary frequencies.

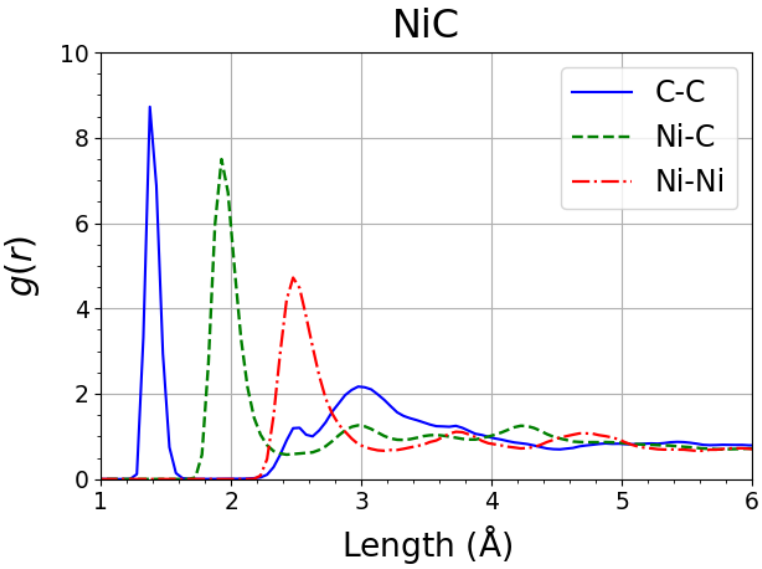


Figure S3: Radial distribution functions *g(r)* of individual bonding pairs within the 5×5×5 supercell of NiC, obtained from molecular dynamics simulations carried out at 300 K. The peaks occurring near 1.4 Å, 1.9 Å, and 2.5 Å correspond to nearest-neighbor C-C, Ni-C, and Ni-Ni bonds respectively. With the exception of some very broad peaks corresponding to second-nearest-neighbor distances, there are no distinct features beyond approximately 3 Å, indicating the loss of long-range order.

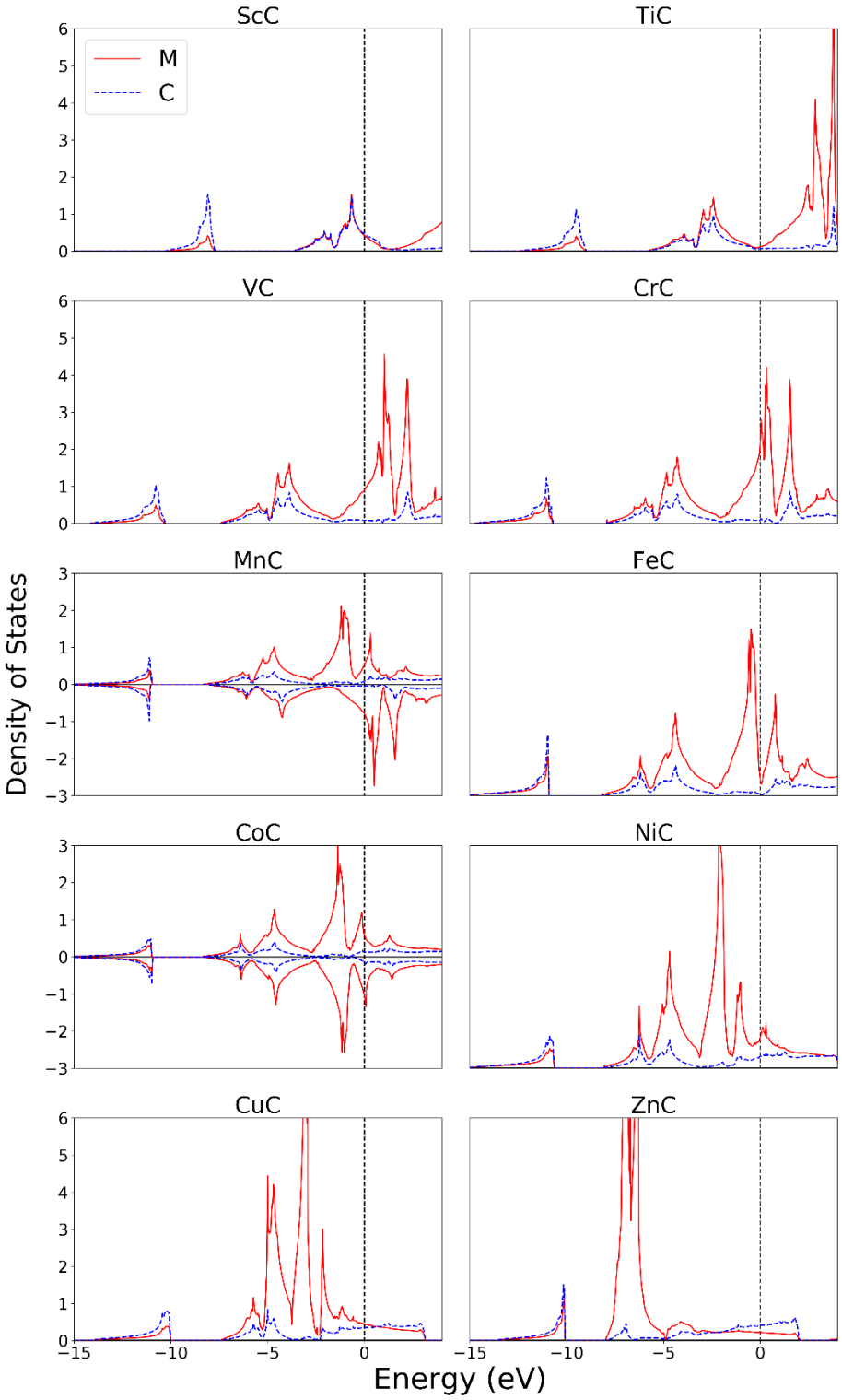


Figure S4: Local density of states (LDOS) of the 3*d* rocksalt TMCs. Metal (M) and carbon (C) densities are plotted separately. The Fermi level is set to 0 eV. For MnC and CoC, which display non-zero magnetization, majority- and minority-spin densities are plotted above and below the x-axis respectively.

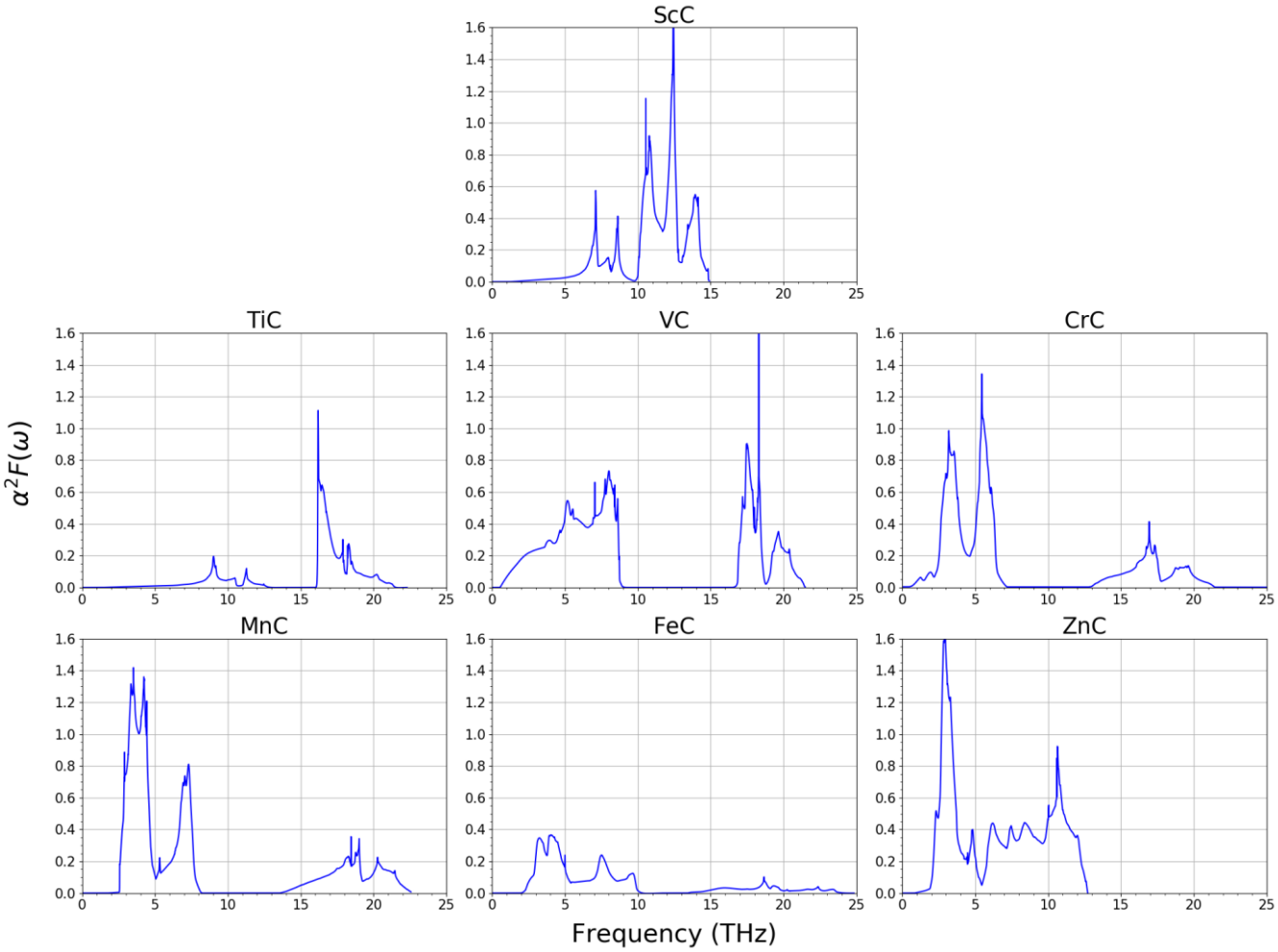
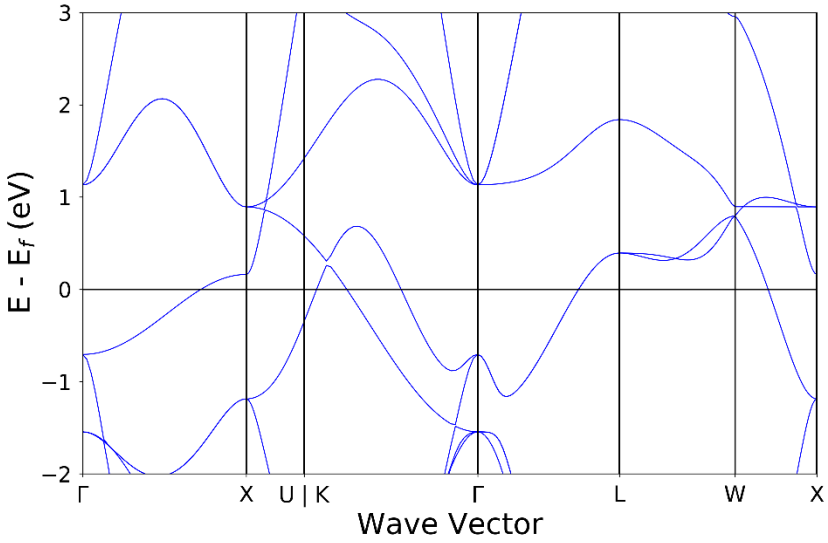


Figure S5: The dimensionless Eliashberg function $\alpha^2F(\omega)$, which relates the contribution of each phonon frequency to the electron-phonon interaction, is shown for all stable rocksalt 3*d* TMCs.

(a)



(b)

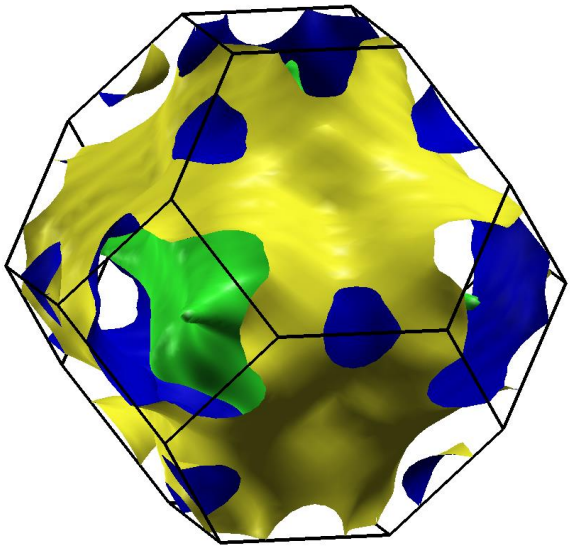


Figure S6: (a) The electronic band structure of CrC, plotted along high-symmetry paths in the Brillouin zone. (b) The Fermi surface of CrC, plotted in the first Brillouin zone, with the inner (green) and outer (blue/yellow) sheets corresponding to individual electronic bands crossing the Fermi level in the band structure.

References

1. D.B. Rogers, *et al.*, Inorg. Chem., 1970, **10**, 723.