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Charge Density Waves and the Hidden Nesting of Purple Bronze KMo6O17[1] LEI SU, VITOR PEREIRA, National University of Singapore — The layered purple bronze KMo_6O_{17}, with its robust triple CDW phase up to high temperatures, became the emblematic example of the "hidden nesting" concept. Recent experiments suggest that, on the surface layers, its CDW phase can be stabilized at much higher temperatures, and with a tenfold increase in the electronic gap in comparison with the bulk. Despite such interesting fermiology and properties, the K and Na purple bronzes remain largely unexplored systems, most particularly so at the theoretical level. We introduce the first multi-orbital effective tight-binding model to describe the effect of electron-electron interactions in this system. Upon fixing all the effective hopping parameters in the normal state against an ab-initio band structure, and with only the overall scale of the interactions as sole adjustable parameter, we find that a self-consistent Hartree-Fock solution reproduces extremely well the experimental behavior of the charge density wave (CDW) order parameter in the full range $0 < T < T_c$, as well as the precise reciprocal space locations of the partial gap opening and Fermi arc development. The interaction strengths extracted from fitting to the experimental CDW gap are consistent with those derived from an independent Stoner-type analysis

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