Pressure dependence of the superconducting transition temperature in 2M-WS_2 and 3R-WS_2 based on the first-principles calculations

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Recently, transition metal dichalcogenide (TMD) 2M-WS_2 with the superconducting transition temperature T_c = 8.8K[1] which is the highest among TMDs has attracted much attention as a promising candidate exhibiting topological surface state and topological superconductivity[2,3]. When pressure is applied, T_c monotonically decreases with increasing pressure down to 3.5K at 18GPa above which the system shows a broad structural transition from 2M phase to 3R phase accompanied by a transition from metal to semiconductor with no superconductivity[4]. Remarkably, when the pressure exceeds 45GPa, 3R-WS_2 shows a metallic behavior and also the superconductivity with T_c = 2.5K which is almost independent of pressure up to 65GPa[4]. Theoretically, T_c in 2M-WS_2 at ambient pressure was estimated from the first-principles calculations to be 2K which is about 1/4 of the experimental value[1]. The pressure dependence of T_c including the high-pressure 3R phase, however, has not been discussed there. In the present paper, we examine the pressure dependence of T_c in both 2M-WS_2 and 3R-WS_2 on the basis of the first-principles calculations with the use of the McMillan formula. In 2M-WS_2, we find that T_c decreases with increasing pressure as observed in the experiments although the values of T_c are about 1/3~1/6 of the experimental values. On the other hand, T_c is estimated to be zero independent of pressure in 3R-WS_2, where the conventional BCS phonon mechanism is considered to fail to account for the superconductivity. We also discuss a possible mechanism of the superconductivity in 3R-WS_2 on the basis of the first-principles calculated Fermi surfaces which show strong nesting between the small electron and hole pockets.

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[2] Y. Yuan et al., Nature Physics **15**, 1046 (2019).
[3] Y. W. Li *et al*., Nature Communications **12**, 2084 (2021).
[4] W. Zhang *et al*., J. Phys. Chem. Lett. **12**, 3321 (2021).