

## Supplemental Material

### Carrier mobility and superconducting properties in monolayer oxygen-terminated functionalized MXene $\text{Ti}_2\text{CO}_2$

Reza Shayanfar,<sup>1</sup> Mohammad Alidoosti,<sup>2</sup> Davoud Nasr Esfahani,<sup>2,3</sup> and Mahdi Pourfath<sup>1,4,\*</sup>

<sup>1</sup>*School of Electrical and Computer Engineering,  
College of Engineering, University of Tehran, Tehran 14395-515, Iran*

<sup>2</sup>*Pasargad Institute for Advanced Innovative Solutions (PIAIS), Tehran 19916-33361, Iran*

<sup>3</sup>*Department of Converging Technologies, Khatam University, Tehran 19916-33357, Iran*

<sup>4</sup>*Institute for Microelectronics/E360, TU Wien, A-1040 Vienna, Austria*

(Dated: October 17, 2023)

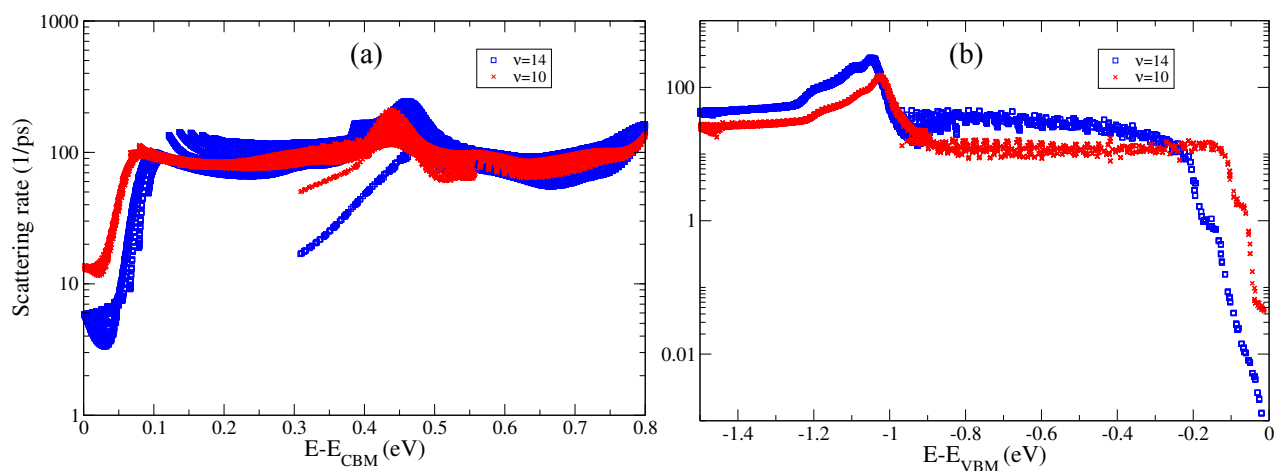


FIG. S1: The scattering rates of the two most effective optical modes ( $\nu = 10$  and 14) as functions of energy for the (a) n- and (b) p-type (0.01 el/cell)  $\text{Ti}_2\text{CO}_2$ . The temperature was assumed to be 300 K.

\*Electronic address: [pourfath@ut.ac.ir](mailto:pourfath@ut.ac.ir)

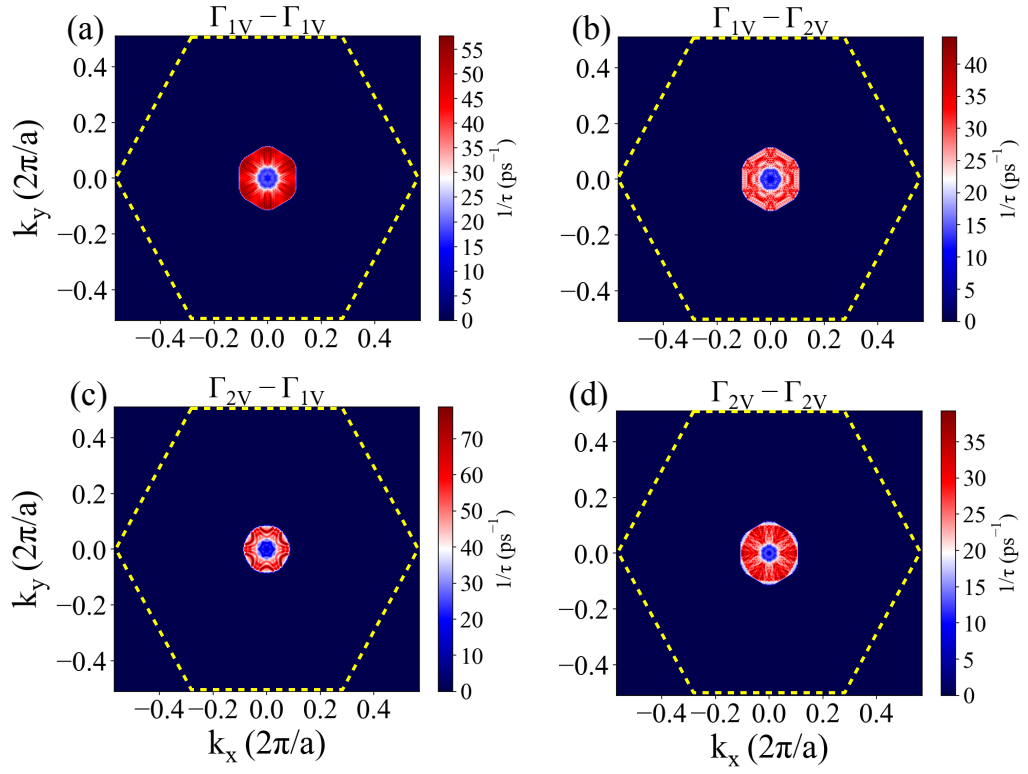


FIG. S2: Valley-dependent hole scattering rates ( $1/\text{ps}$ ). Hole concentration and temperature are assumed to be 0.01 el/cell and 300 K, respectively. The possible intra/inter-valley transitions are illustrated in (a-d).

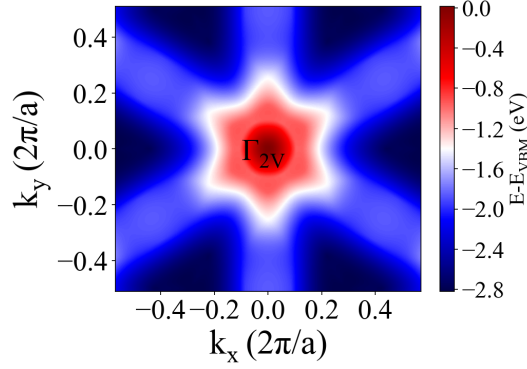


FIG. S3: The Fermi surface of the valence band consisting of  $\Gamma_{2V}$  valley.

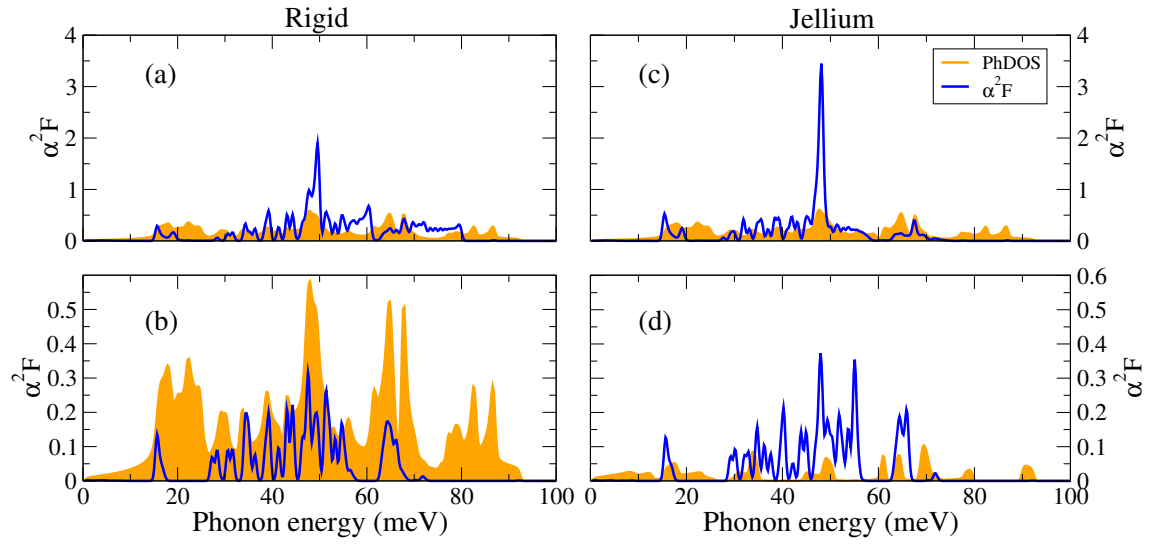


FIG. S4: Isotropic Eliashberg spectral function ( $\alpha^2 F$ ) and phonon density of states (PhDOS) for monolayer  $\text{Ti}_2\text{CO}_2$  within both the rigid and the jellium regimes. The rigid band  $\alpha^2 F$  and PhDOS of (n-type) -0.01 el/cell (a) and (p-type) +0.01 el/cell (b) are illustrated. (c) and (d) are the same as (a) and (b) except in the jellium regime.