

Supporting information

Theoretical study on pseudo Mott phase transition of vanadium dioxide

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Table S-1 Comparison of stability of spin-polarized and spin-unpolarized R and M₁ phases.

$E(\text{eV})$	spin-polarization (R)	spin-polarization (M ₁)	spin-unpolarization (R)	spin-unpolarization (M ₁)
$U=2$	-151.49	-151.33	-150.72	-150.93
$U=0$	-144.52	-144.62	-142.59	-143.21

Potential energy surface with linear interpolation

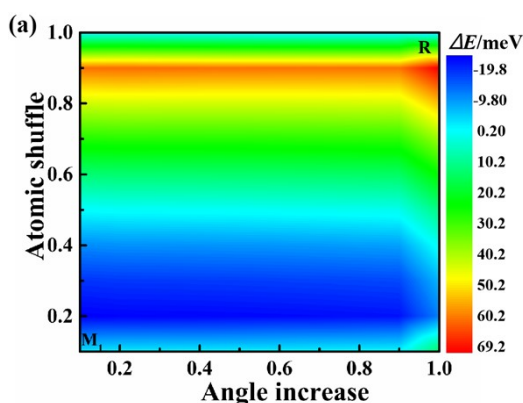


Figure S-1 Potential energy surface of cell shear from M₁ to R phase.

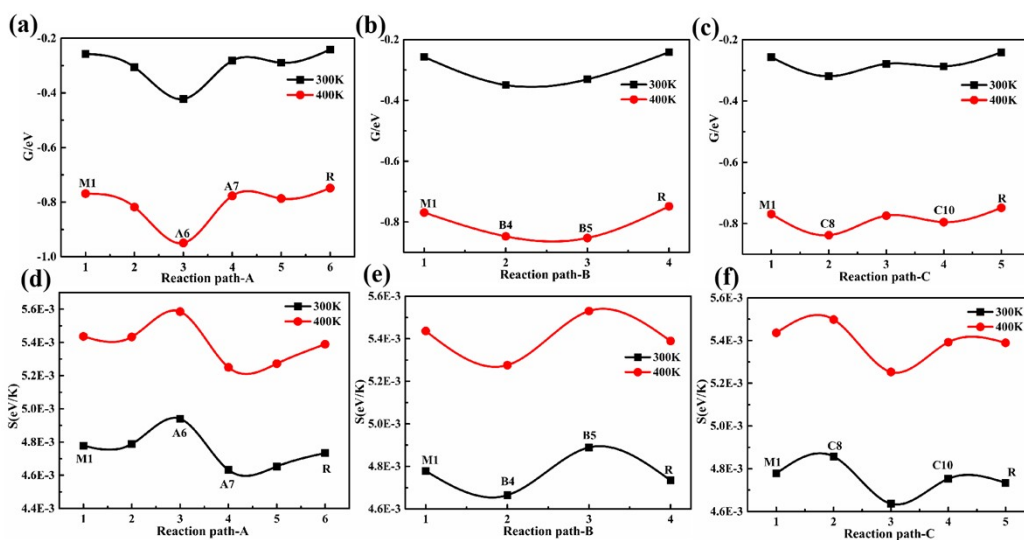


Figure S-2 Free energies and vibrational entropies of several structures at 300 and 400 K along the path A, B and C.

Evolution of electronic and geometrical structure

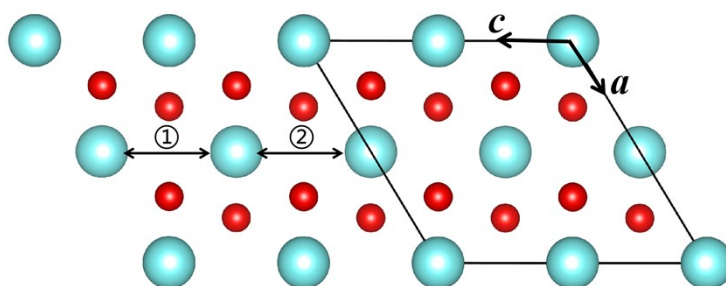


Figure S-3 Variation of V-V distances. Red spheres represent oxygen atoms while the others represent vanadium atoms.

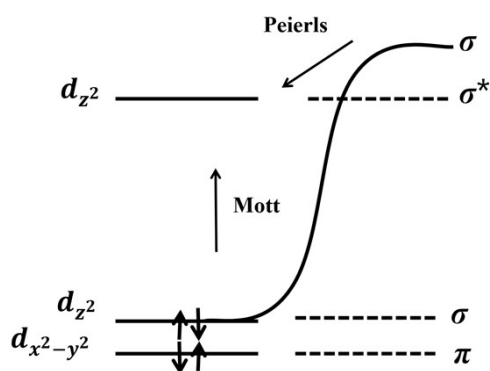


Figure S-4 Schematic diagram of electron orbitals for Peierls transition and Mott transition.

From hole to electron carriers

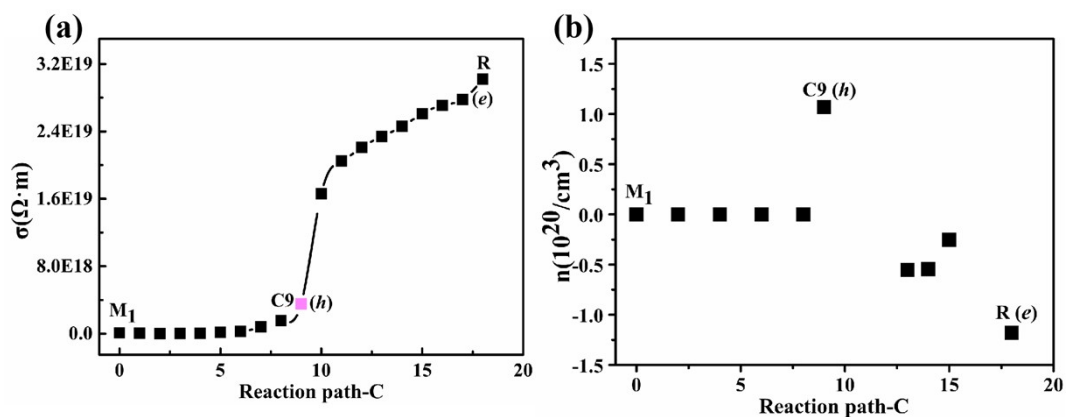


Figure S-5 Theoretical conductivity (a) and carrier concentrations (b) along the path C.