Supporting Information

$Na_2Cu_2TeO_6$: A Potential Material for High Solar Cell Efficiency and Superior Energy-Harvesting Performance

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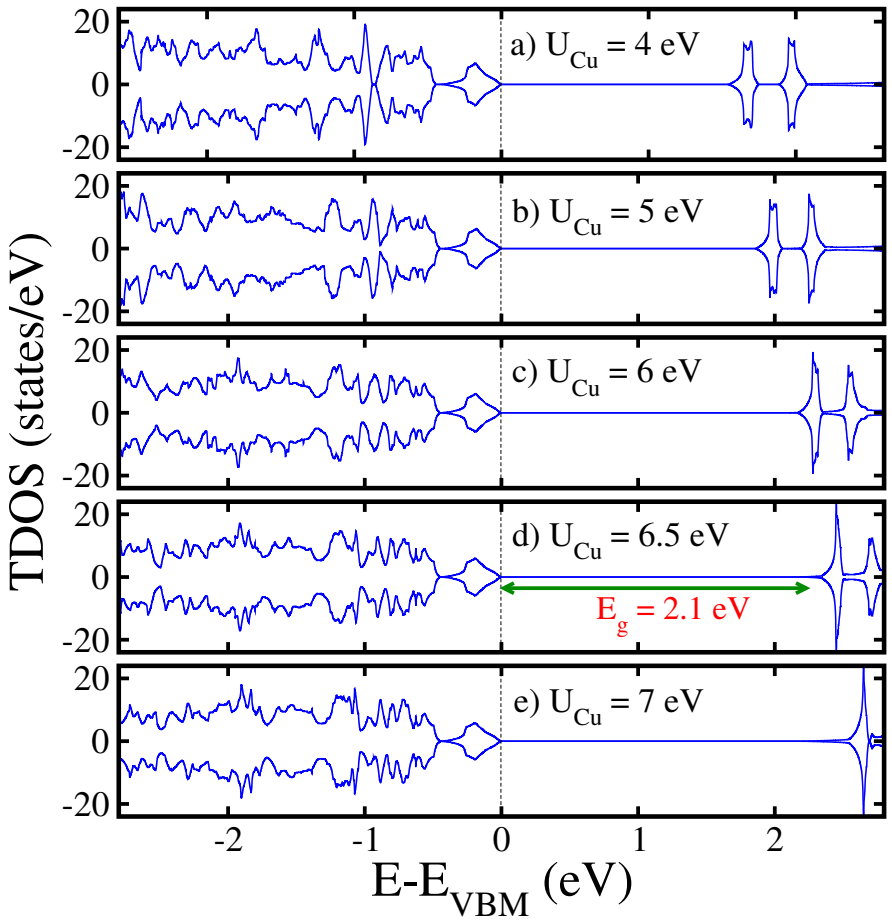

FIG. 1S: GGA+U calculated spin-polarized total density of states (TDOS) for U = (a) 4, (b) 5, (c) 6, (d) 6.5, and (e) 7 eV for the $Na_2Cu_2TeO_6$ material in the stable antiferromagnetic state.

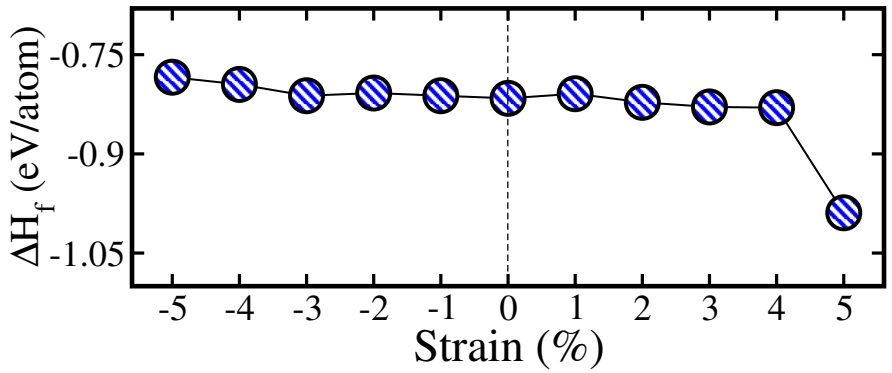

FIG. 2S: GGA+U calculated formation enthalpy (ΔH_f) for the $Na_2Cu_2TeO_6$ material against ±5% biaxial ([110]) strain.

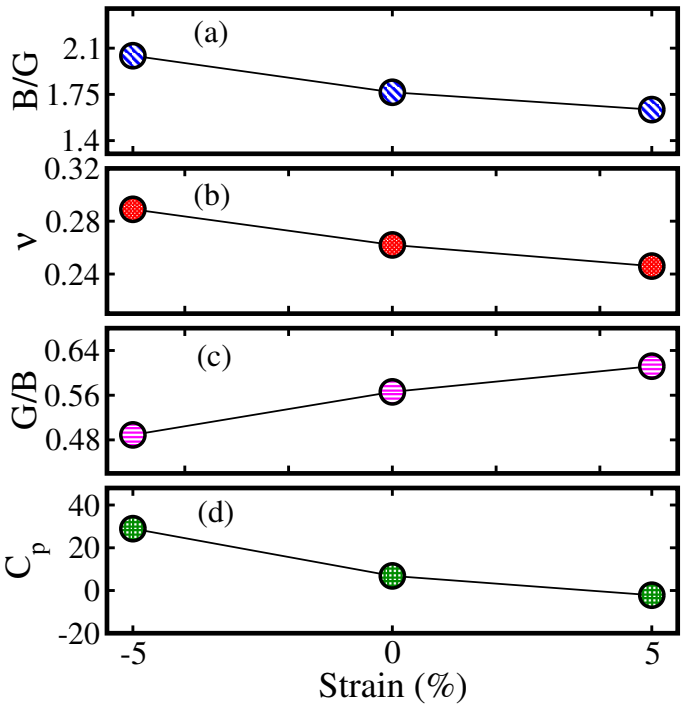

FIG. 3S: Computed (a) Pugh's ratio ($\frac{B}{G}$), (b) Poisson's ratio (ν), (c) $\frac{G}{B}$, (d) Cauchy's pressure (C_p) of the $Na_2Cu_2TeO_6$ material under $-5\%/0\%/+5\%$ strain.

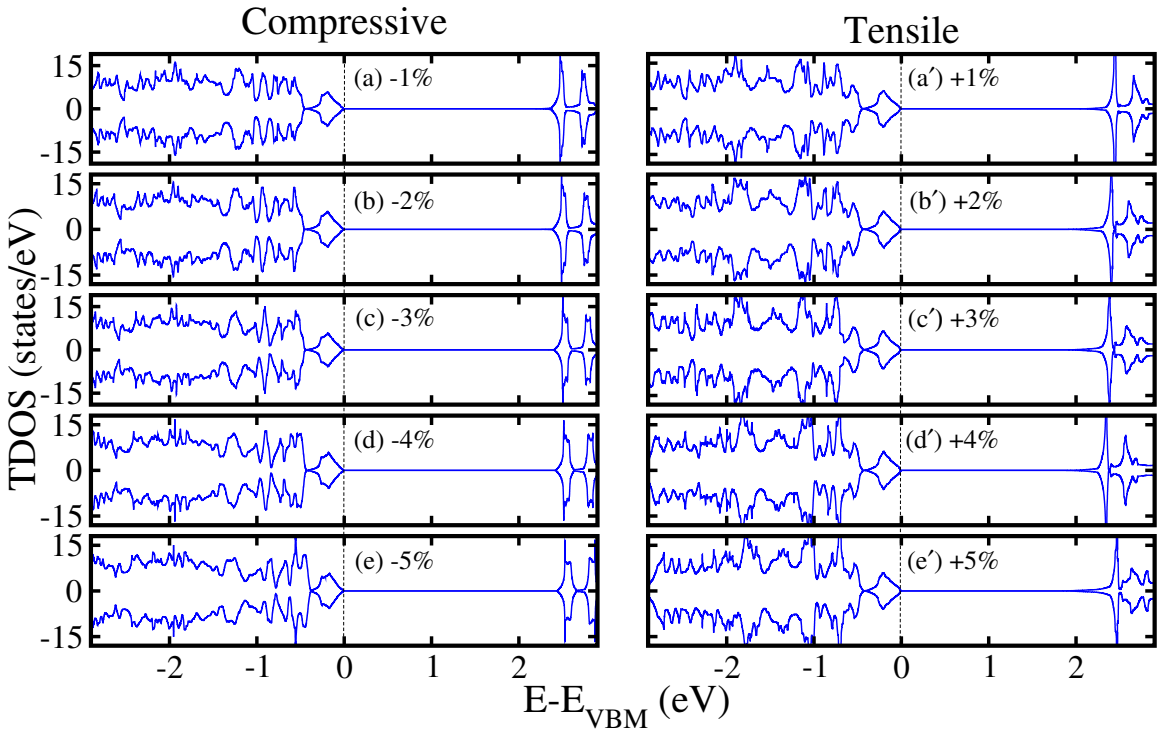

FIG. 4S: GGA+U calculated spin-polarized total density of states (TDOS) under compressive/tensile strain for the (a/a′) $-1/+1\%$, (b/b′) $-2/+2\%$, (c/c′) $-3/+3\%$, (d/d′) $-4/+4\%$, and (e/e′) $-5/+5\%$ of the $Na_2Cu_2TeO_6$ material in the stable antiferromagnetic state.

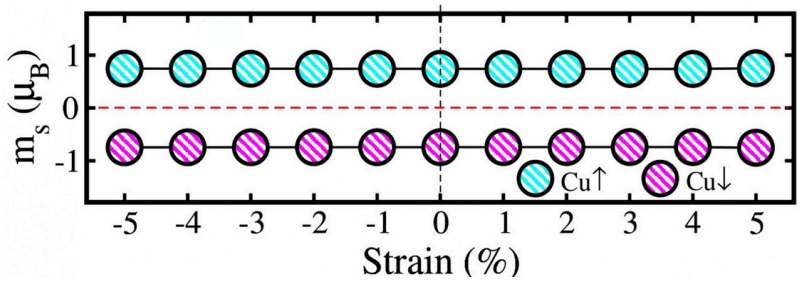

FIG. 5S: GGA+U calculated local spin magnetic moment (m_s) on the Cu ions of the $Na_2Cu_2TeO_6$ material against $\pm 5\%$ biaxial ([110]) strain.

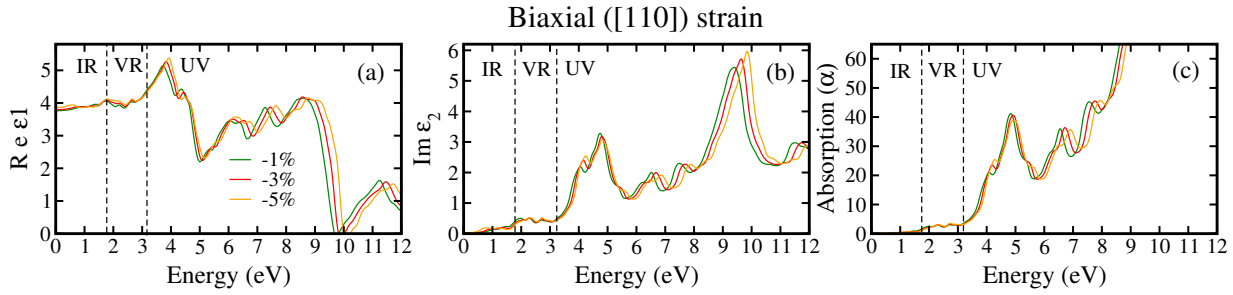

FIG. 6S: Calculated various optical parameters such as (a) real dielectric part ($\epsilon_1(\omega)$), (b) imaginary dielectric part ($\epsilon_2(\omega)$), and (c) absorption coefficient ($\alpha(\omega)$) in 10^4 cm^{-1} under $-1\%/-3\%/-5\%$ biaxial ([110]) strain for the $Na_2Cu_2TeO_6$ material.