Optoelectronic properties of TiS_2: a never ended story tackled by density functional theory and many body methods

Adrien Stoliaroff, Stéphane Jobic, Camille Latouche*
*camille.latouche@cnrs-imn.fr
Institut des matériaux Jean Rouxel – Université de Nantes, CNRS, 2 rue de la Houssinière, BP 32229, 44322 Nantes Cedex 3, France

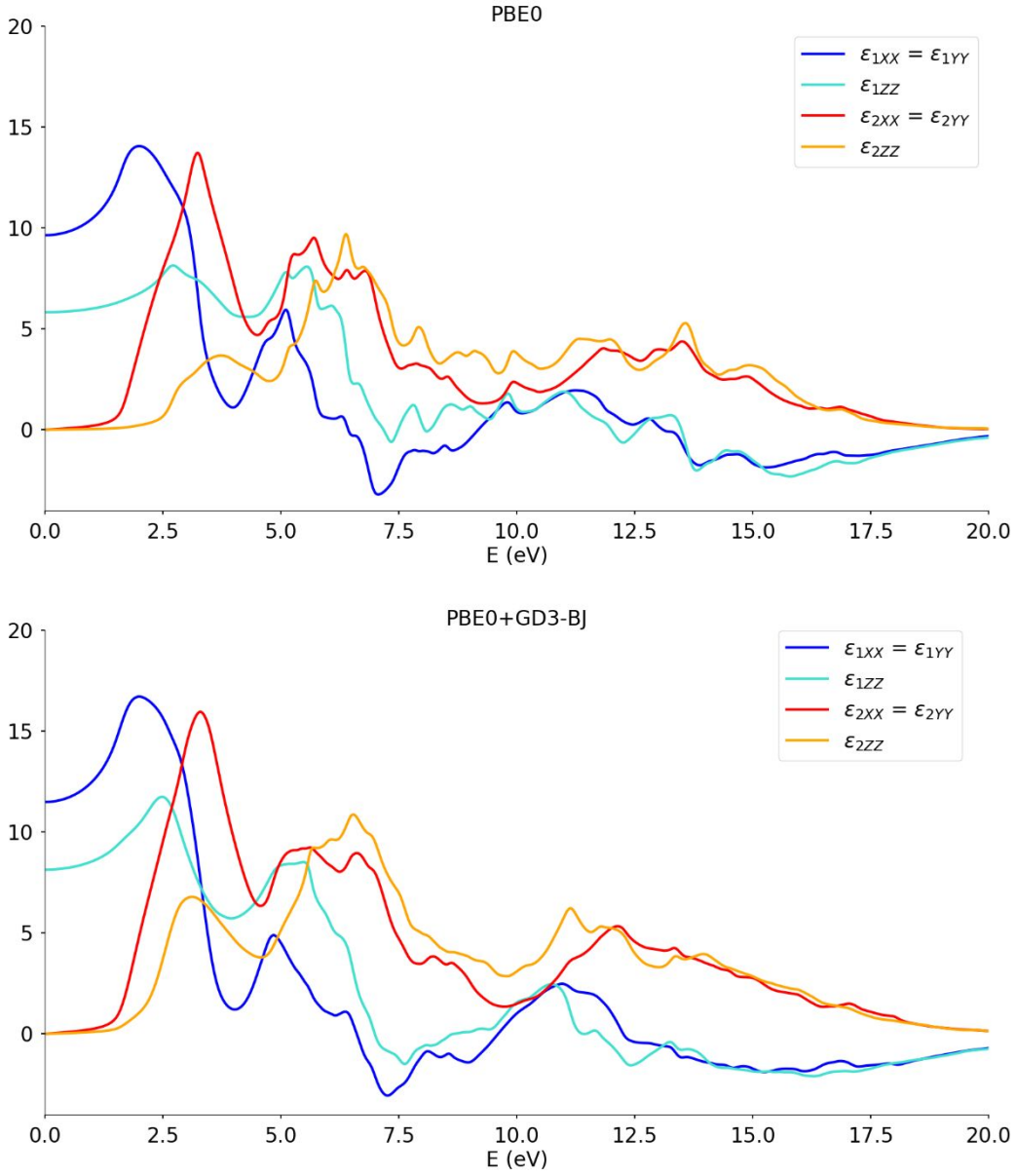

Figure S1. Simulated ε_1, ε_2 optical indices enforcing PBE0 and PBE0-D levels of theory.

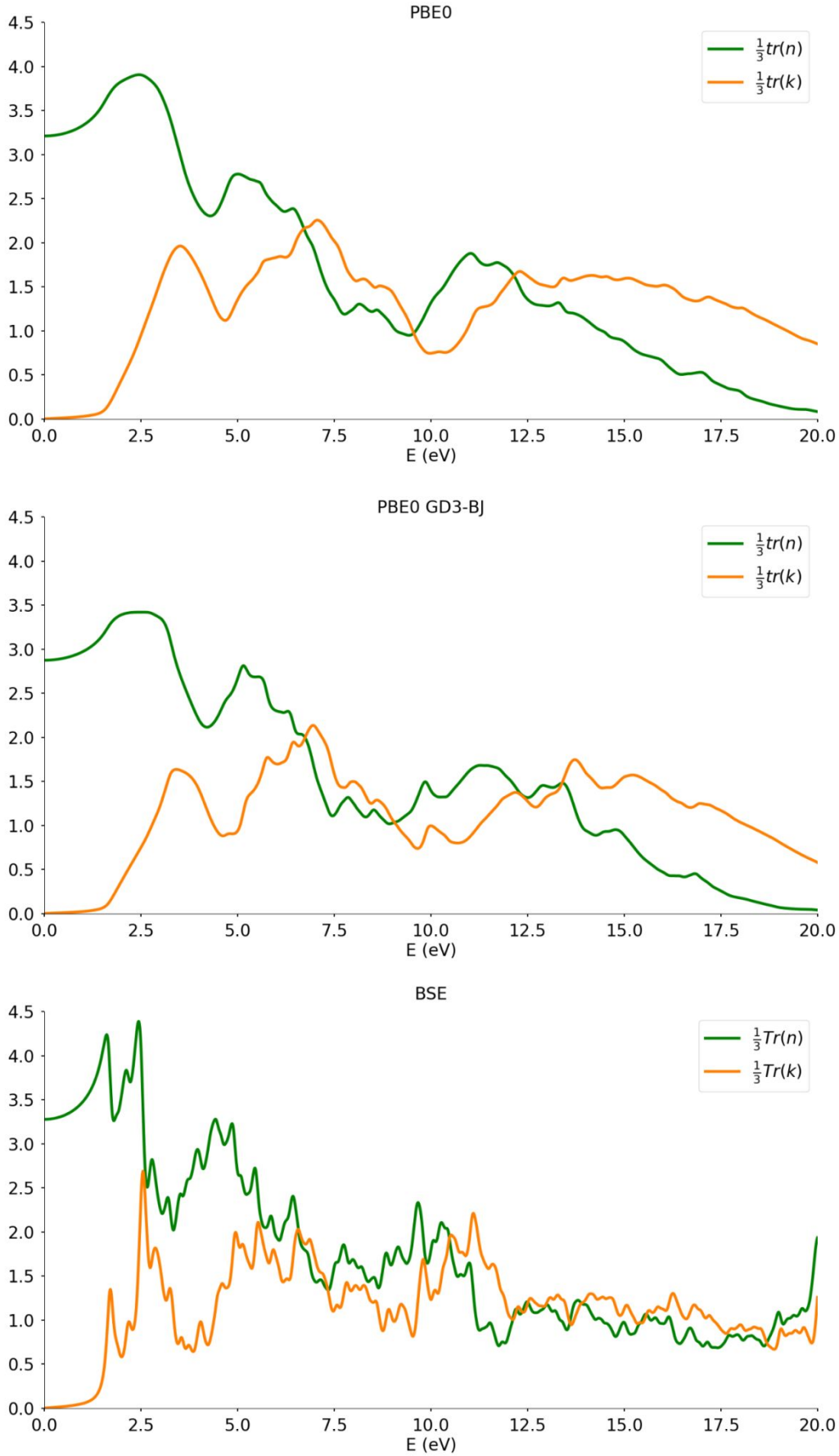

Figure S2. Simulated *n, k* optical indices enforcing PBE0, PBE0-D and BSE levels of theory.

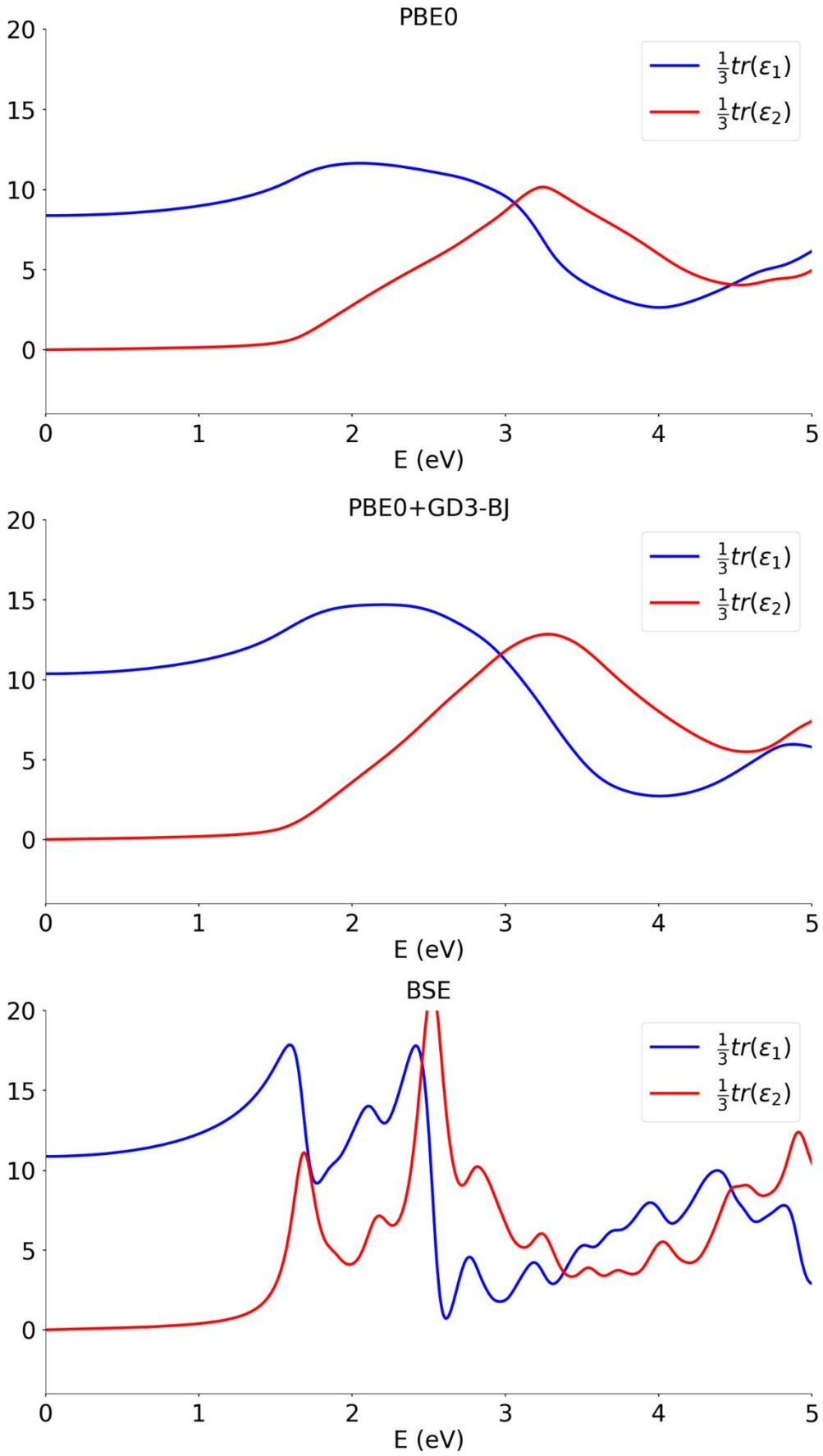

Figure S3. Simulated ε_1, ε_2 optical indices enforcing PBE0, PBE0-D and BSE levels of theory.

In this case, as $\boldsymbol{\varepsilon_{xx} = \varepsilon_{yy}}$, $\boldsymbol{\frac{1}{3}tr(\varepsilon) = \varepsilon_{iso} = \frac{2}{3}\varepsilon_{xx} + \frac{1}{3}\varepsilon_{zz}}$.