SUPPORTING INFORMATION

Effect of Ligand Groups on Photoexcited Charge Carrier Dynamics at Perovskite/TiO_2 Interface

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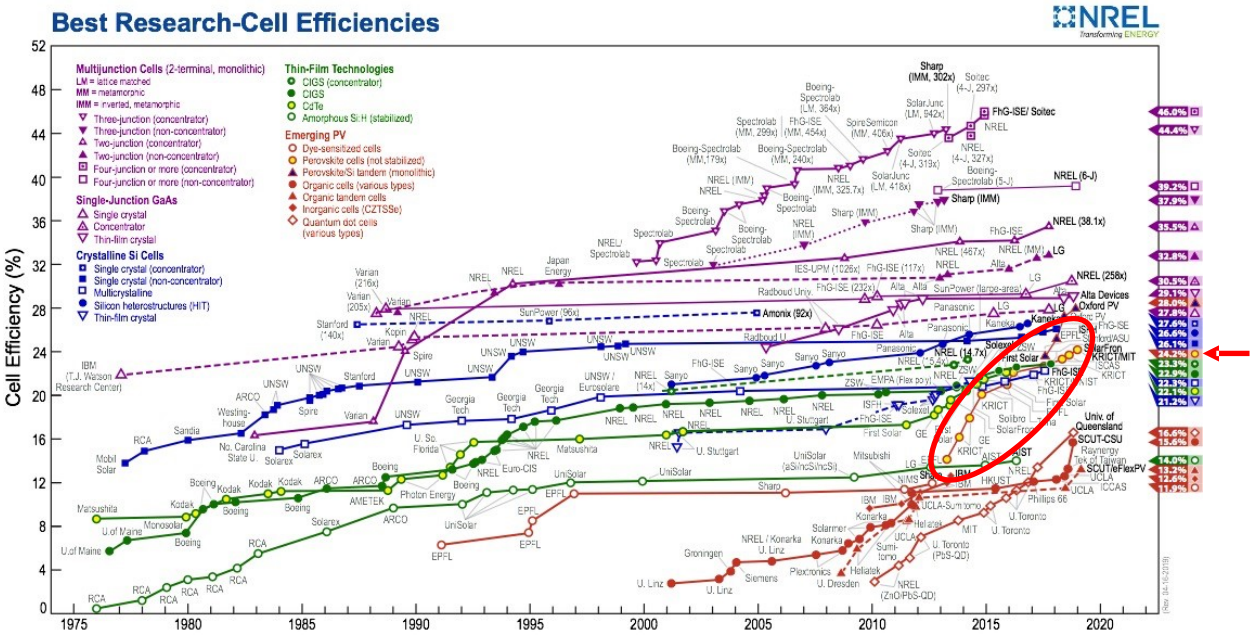

Figure S1. Plot of highest verified solar cell efficiencies vs time. Perovskite solar cells are circled and the current maximum perovskite solar cell efficiency is pointed out on the right. The plot was taken from https://www.nrel.gov/pv/cell-efficiency.html

The Fock matrix is defined as:

$$F = \sum_{i}^{n_e/2}\left(h_i + \sum_{j=1}^{n_e/2}\left[2J_j - K_j\right]\right) \tag{S1}$$

Where h_i is the one-electron Hamiltonian for the i^{th} orbital,

$$J_j(\vec{r}) = \int d\vec{r}' \frac{\left|\varphi_j(\vec{r}')\right|^2}{|\vec{r} - \vec{r}'|} \tag{S2}$$

Is the Coulomb operator, and

$$K_j(\vec{r})\varphi_i(\vec{r}) = \varphi_j(\vec{r}) \int d\vec{r}' \frac{\varphi_j^*(\vec{r}')\varphi_i(\vec{r}')}{|\vec{r} - \vec{r}'|} \tag{S3}$$

Is the action of the exchange operator on an orbital $\varphi_i(\vec{r})$.