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:

$$ F = \sum_{i} \frac{n_i}{2} \left[ \hat{h}_i + \sum_{j=1}^{n_i} (2\hat{J}_j - \hat{K}_j) \right] $$

(S1)
Where $h_i$ is the one-electron Hamiltonian for the $i^{th}$ orbital,

$$J_j(\vec{r}) = \int d\vec{r}' |\phi_j(\vec{r}')|^2 \frac{1}{|\vec{r} - \vec{r}'|}$$

(S2)

Is the Coulomb operator, and

$$K_j(\vec{r})\phi_i(\vec{r}) = \phi_j(\vec{r}) \int d\vec{r}' \phi_j^*(\vec{r}') \phi_i(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|}$$

(S3)

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