Negativity of the target density in practical Frozen-Density Embedding Theory based calculations

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Abstract

Tentative abstract

1 Introduction

- $E^{FDET}_{v_A,v_B}[\Psi_A,\rho_B] = \langle\Psi_A|\hat{H}_A|\Psi_A\rangle + E^{HK}_{v_B}[\rho_B] + E^{int}_{v_A,v_B} + \Delta F[\rho_A] + \int\rho_A(\vec{r})v_B(\vec{r})d\mathbf{r} + \int\int\frac{\rho_A(\vec{r})\rho_B(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'d\mathbf{r} + E^{nad}_{xcT}[\rho_A,\rho_B] + \int\rho_B(\vec{r})v_A(\vec{r})d\mathbf{r}$
- $E^{FDET}_{v_A,v_B}[\Psi^o_A,\rho_B] = E^{HK}_{v_{AB}}[\rho^o_A+\rho_B] \geq E_o$
- if $\rho^t(\mathbf{r}) = \rho_o(\mathbf{r}) - \rho_B(\mathbf{r})$ is not positive for $\forall\mathbf{r}$, then it is not v-representable, and there is no possible embedding potential that can lead to $\rho^t(\mathbf{r})$
- the aim of this manuscript is to assess if there is a relation between some measurement of the negativity of $\rho^t(\mathbf{r})$ and $E^{FDET}_{v_A,v_B}[\Psi_A,\rho_B]$
- polarization and charge transfer can be expected to influence the extent of violation of the target density. This manuscript also aims at assessing the relation between negativity of the target density and phenomena such as polarization and charge transfer

- Why these 4 systems

$$a = \frac{\delta E^{nad}_{xcT}[\rho_A, \rho_B]}{\delta \rho_A(\mathbf{r})}\Big|_{\rho_A=\rho_A^{ref}} \tag{1}$$

Graphical TOC Entry

TOC to be made. Probably isosurfaces of target density.