

Quantitative Current-Voltage Characteristics in Molecular Junctions from First Principles: Supplementary Information

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Abstract

Supplementary Information for the manuscript “Quantitative Current-Voltage Characteristics in Molecular Junctions from First Principles”. Experimental Methods, level alignment and self-energy corrections, analytical changes in the density of a Lorentzian model, basis sets, geometries, plot of the self-consistent density matrices, Hartree potentials and transmission functions at finite biases are reported.

Contents

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Experimental Methods

We form single-molecule junctions by breaking a gold point contact in a solution of the molecules (Xu, B. Q.; Tao, N. J. *Science*, **2003**, 301, 1221-1223) and measure the conductance while pulling the junction apart at a constant speed of 16 nm s^{-1} . Details of our experimental set-up have been described previously (Venkataraman, L.; Klare, J. E.; Nuckolls, C.; Hybertsen, M. S.; Steigerwald, M. L. *Nature*, **2006**, 442, 904-907; Widawsky, J. R. et al. *Nanotechnology*, **2009**, 20, 434009). The measurements are carried out at room temperature, in ambient conditions. A bias (V_A) is applied across the junction and series resistor. We measure the bias (V_M) across the tip-substrate junction and determine the conductance ($\mathcal{G} = I/V_M$) by dividing the measured current with the measured voltage. For single-molecule-junction $I(V)$ measurements, the STM tip is brought into contact with the Au substrate until a conductance of greater than a few G0 is obtained at an applied bias of about 50 mV. The tip is then withdrawn. This distance is chosen to ensure that the gold point contact is broken by the end of this elongation, a prerequisite for forming a molecular junction. At this point, the tip-substrate distance is held constant for about 150 ms. During this 'hold' period, the V_A is ramped sinusoidally for one period and the current is measured. At the end of this ramp, V_A is set to 50 mV once again and the tip is withdrawn an additional 2.4 nm to fully break the junction.

Level Alignment and Self-energy corrections

Energies of the HOMO-LUMO are obtained through the diagonalization of the junction Hamiltonian on the subspace generated by the numerical orbitals of the atoms belonging to the molecule. Self-energy corrections are reported in table Table 1.

Table 1: Energy of the HOMO (LUMO) for the 4 molecules in the gas-phase constrained in the position of the junctions (GP), in the junctions (J) with adatom-adatom/adatom-trimer/trimer-trimer (BP–Asym was only considered in the adatom-trimer geometry), and corresponding self-energy (SE) corrections. Gas-phase energies are given with respect to the vacuum energy. Junctions energy are given wrt to the junction Fermi energy (-4.55eV). Differences in the DFT-PBE GP and Σ for different binding sites (not reported here) are smaller than 0.05eV for DFT-PBE GP and 0.02eV for Σ

Molecule/ Junction	DFT-PBE GP [eV]	DFT-PBE Junction [eV] <i>ad-ad/ad-trim/trim-trim</i>	Σ_{GP} [eV]	Σ_{CORR} [eV]	$\Sigma = \Sigma_{\text{GP}}$ $+ \Sigma_{\text{CORR}}$ [eV]
APA	-4.38 (-1.67)	-0.90/-0.88/-0.87 (1.94)/(1.95)/(1.96)	-2.32 (1.61)	0.68 (-0.65)	-1.64 (0.96)
	-5.95 (-2.84)	-3.41/-3.36 /-3.31 (0.28)/(0.38)/(0.46)	-3.19 (2.19)	1.07 (-0.99)	-2.12 (1.20)
BP	-6.03 (-3.01)	-3.0 (<i>ad-trim</i>) (0.25) (<i>ad-trim</i>)	-3.03 (2.17)	1.24 (-1.11)	-1.79 (1.06)
	-4.24 (-1.83)	-0.73/-0.70/-0.68 (1.80)/(1.83)/(1.85)	-2.25 (1.70)	0.67 (-0.63)	-1.58 (1.07)
DAS	-5.14 (0.86)	-3.55/-3.46/-3.38 (4.01)/(4.05)/(4.15)	-3.03 (-0.41)	1.03 (-0.89)	-2.00 (-1.30)

Changes in the density at Finite-Bias in a Lorentzian model

Definitions

$$\Delta\rho = \rho(V) - \rho(0) \quad (1)$$

$$\rho(V) = \frac{-i}{2\pi} \int_{-\infty}^{+\infty} d\omega \mathcal{G}^<(\omega; V) \quad (2)$$

$$\rho(0) = \frac{-i}{2\pi} \int_{-\infty}^{+\infty} d\omega \mathcal{G}^<(\omega; V=0) \quad (3)$$

$$\mathcal{G}^<(\omega; V) = i\mathcal{G}^r(\omega; V) \left(f_{\text{FD}} \left(\omega - \frac{|V|}{2} \right) \Gamma_L + f_{\text{FD}} \left(\omega + \frac{|V|}{2} \right) \Gamma_R \right) \mathcal{G}^a(\omega; V) \quad (4)$$

Lorentzian Model:

$$\Gamma_L = |\Psi\rangle\Gamma_L\langle\Psi| \quad (5)$$

$$\Gamma_R = |\Psi\rangle\Gamma_R\langle\Psi| \quad (6)$$

$$\mathcal{G}^r(\omega; V) = \frac{|\Psi\rangle\langle\Psi|}{\omega - E(V) - i\Gamma} \quad (7)$$

$$\mathcal{G}^a(\omega; V) = \frac{|\Psi\rangle\langle\Psi|}{\omega - E(V) + i\Gamma} \quad (8)$$

Symmetric:

$$\Gamma_L = \Gamma_R = \frac{\Gamma}{2} \quad (9)$$

$$E(V) \simeq E \quad (10)$$

$$\mathcal{G}^r(\omega; V) \simeq \mathcal{G}^r(\omega; V=0) \quad (11)$$

$$\mathcal{G}^a(\omega; V) \simeq \mathcal{G}^a(\omega; V=0) \quad (12)$$

Derivation

$$\Delta\rho = \frac{-i}{2\pi} \int_{-\infty}^{+\infty} d\omega [\mathcal{G}^<(\omega; V) - \mathcal{G}^<(\omega; V=0)] \quad (13)$$

$$= \frac{\Gamma}{2\pi} \int_{-\infty}^{+\infty} d\omega \mathcal{G}^r(\omega) \left[f_{\text{FD}}\left(\omega - \frac{|V|}{2}\right) + f_{\text{FD}}\left(\omega + \frac{|V|}{2}\right) - 2f_{\text{FD}}(\omega) \right] \mathcal{G}^a(\omega) \quad (14)$$

$$= \frac{\Gamma}{2\pi} \int_{-\infty}^{+\infty} d\omega \mathcal{G}^r(\omega) \mathcal{F}(\omega) \mathcal{G}^a(\omega) \quad (15)$$

$$\mathcal{F}(\omega) = f_{\text{FD}}\left(\omega - \frac{|V|}{2}\right) + f_{\text{FD}}\left(\omega + \frac{|V|}{2}\right) - 2f_{\text{FD}}(\omega) \quad (16)$$

$$\mathcal{F}(\omega) = 1 \text{ for } \omega \in \left[0; \frac{|V|}{2}\right] \quad (17)$$

$$\mathcal{F}(\omega) = -1 \text{ for } \omega \in \left[-\frac{|V|}{2}; 0\right] \quad (18)$$

$$\mathcal{F}(\omega) = 0 \text{ otherwise} \quad (19)$$

$$\rho(0) = \frac{1}{\Gamma\pi} \int_{-\infty}^0 d\omega \frac{1}{\left(\frac{\omega-E}{\Gamma}\right)^2 + 1} \quad (20)$$

$$= \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{E}{\Gamma}\right) \quad (21)$$

and

$$\Delta\rho = \frac{\Gamma}{2\pi} \left[\int_{-\frac{|V|}{2}}^0 d\omega \frac{-1}{(\omega-E)^2 + \Gamma^2} + \int_0^{\frac{|V|}{2}} d\omega \frac{1}{(\omega-E)^2 + \Gamma^2} \right] \quad (22)$$

$$= \frac{1}{2\Gamma\pi} \left[\int_{-\infty}^{\frac{|V|}{2}} d\omega \frac{1}{\left(\frac{\omega-E}{\Gamma}\right)^2 + 1} + \int_{-\infty}^{-\frac{|V|}{2}} d\omega \frac{1}{\left(\frac{\omega-E}{\Gamma}\right)^2 + 1} - 2 \int_{-\infty}^0 d\omega \frac{1}{\left(\frac{\omega-E}{\Gamma}\right)^2 + 1} \right] \quad (23)$$

$$= \frac{1}{2\pi} \left[\arctan\left(\frac{\frac{V}{2}-E}{\Gamma}\right) + \arctan\left(\frac{-\frac{V}{2}-E}{\Gamma}\right) + 2\arctan\left(\frac{E}{\Gamma}\right) \right] \quad (24)$$

This equation leads to a maximal correction of $0.007 e^-$ in the case of the bypiridine junction ($E = 1.53 eV$; $\Gamma = \frac{0.068}{2} eV$).

Deviation from the linear response is given by: $\Delta\rho(V) - V \times \left.\frac{\partial\rho}{\partial V}\right|_{V=0}$. In figure 2, we calculate $\left.\frac{\partial\rho}{\partial V}\right|_{V=0}$ by finite differences at $-100 mV$.

$$\Delta\rho(V) - \frac{V}{V_0 = -100mV} \Delta\rho(V_0 = -100mV) \simeq 0.001 e^- \text{ at } V = 1V \quad (25)$$

Interestingly for BP junctions (Fig. 2), where the transmission function is well reproduced

by a Lorentzian expression, the DFT-PBE(V) densities and Hartree potentials remain in the linear response regime to 1V, even though the DFT-PBE level alignment erroneously predicts that the LUMO resonance enters the bias window, suggesting significant charging and a predicted change in occupation of $0.49 e^-$ according to this non-self-consistent model. This indicates that self-consistent DFT-PBE is nonetheless accurate for the prediction of the densities under bias, despite its reliance on DFT-PBE energy level alignment.

Basis set

PAO.BasisType split # Type of PAO basis set

%block PAO.Basis # Define Basis set

C 2 # Species label, number of l-shells

n=2 0 2 # n, l, Nzeta

4.870 3.475

1.000 1.000

n=2 1 2 P 1 # n, l, Nzeta, Polarization, NzetaPol

6.099 3.699

1.000 1.000

H 1 # Species label, number of l-shells

n=1 0 2 P 1 # n, l, Nzeta, Polarization, NzetaPol

5.752 4.002

1.000 1.000

N 2 # Species label, number of l-shells

n=2 0 2 # n, l, Nzeta

4.280 2.905

1.000 1.000

n=2 1 2 P 1 # n, l, Nzeta, Polarization, NzetaPol

```

5.360 3.092
1.000 1.000
Au 2 # Species label, number of l-shells
n=6 0 2 P 1 # n, l, Nzeta, Polarization, NzetaPol
10.544 5.7976
1.000 1.000
n=5 2 1 # n, l, Nzeta
7.811
1.000
%endblock PAO.Basis

```

Geometries

We relax all junctions using DFT within GGA (PBE) as implemented in SIESTA (Ordejón, P.; Artacho, E; Soler, J. M. *Physical Review B*, **1996**, 53, 10441(R); Soler, J. M. et al. *Journal of Physics: Condensed Matter*, **2002**, 14, 2745). Details of our DFT calculations follow those given in Quek, S. Y.; Venkataraman, L.; Choi, H. J.; Louie, S. G.; Hybertsen, M. S.; Neaton, J. B. *Nano Letters*, **2007**, 7, 3477. Hellmann-Feynman forces are optimized to within 0.04eV/Å using GGA-PBE functional and a double- ζ -basis set. We model our system by 7-layers of 16 gold atoms on both sides, the last 4 layers being constrained in the bulk geometry.

APA, AdAtom AdAtom

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APA, Trimer AdAtom

254 ; **C** 9.221556 12.041822 34.162510 ; **C** 9.231025 12.067169 32.726907 ; **C** 8.725024
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258 ; **C** 9.226747 12.041674 34.163686 ; **C** 9.235892 12.066931 32.727538 ; **C** 8.730699
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 8.059504 5.168420 7.311407 ; **Au** 9.551492 11.198259 12.185174 ; **Au** 9.551491 9.475451
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Au 12.535491 4.307015 9.748708 ; **Au** 12.535491 2.584212 7.311395 ; **Au** 11.043487 8.614048
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 12.535491 11.198259 12.185163 ; **Au** 12.535492 9.475447 9.748713 ; **Au** 12.535491 7.752629
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 18.503473 9.475447 9.748721 ; **Au** 18.503472 7.752628 7.311403 ; **Au** 10.451417 20.933519
 52.051092 ; **Au** 10.451413 22.656314 54.487519 ; **Au** 10.451413 24.379131 56.924845 ; **Au**
 8.959429 18.349311 52.051084 ; **Au** 8.959425 20.072109 54.487532 ; **Au** 8.959419 21.794916
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 10.451413 19.210708 56.924843 ; **Au** 8.959425 13.180869 52.051078 ; **Au** 8.959426 14.903678
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 7.467428 22.656318 54.487527 ; **Au** 7.467424 24.379131 56.924852 ; **Au** 5.975425 18.349312
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BP, AdAtom AdAtom

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BP, Trimer AdAtom

248 ; **C** 7.237287 11.381305 26.767284 ; **C** 5.025841 7.227646 30.809387 ; **C** 7.302338
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BP, Trimer AdAtom, Asymmetric Geometry for Linear Stark Correction

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 6.442373 14.613907 27.883877 ; **C** 7.567057 12.585703 26.838146 ; **C** 6.263473 16.024663
 27.916949 ; **C** 8.723408 11.978109 26.275902 ; **C** 5.253413 16.591513 28.704225 ; **H**
 10.787737 14.517316 26.158870 ; **H** 3.836912 13.942234 29.998659 ; **H** 8.864763 15.710709
 27.064225 ; **H** 5.540752 12.807444 28.692731 ; **H** 6.758932 11.956025 27.117505 ; **H** 6.874729
 16.668017 27.368052 ; **H** 8.774832 10.920514 26.217437 ; **H** 5.129002 17.641565 28.762157 ;

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BP, Trimer Trimer

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DAS, Trimer AdAtom

258 ; **C** 9.740342 11.442158 29.518745 ; **C** 9.155190 12.567845 30.171587 ; **C** 8.624950
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260 ; **C** 9.739376 11.445196 29.521558 ; **C** 9.153084 12.570236 30.173951 ; **C** 8.622515
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HDA, AdAtom AdAtom

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HDA, Trimer AdAtom

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HDA, Trimer Trimer

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53.179349 ; **Au** 1.491989 21.340215 48.305585 ; **Au** 1.491992 23.063010 50.742020 ; **Au**
1.491993 24.785816 53.179342 ; **Au** 0.000001 18.755996 48.305589 ; **Au** 0.000001 20.478805
50.742014 ; **Au** -0.000001 22.201600 53.179332 ; **Au** 1.491984 16.171773 48.305586 ; **Au**
1.491992 17.894592 50.742032 ; **Au** 1.491992 19.617390 53.179342 ; **Au** 0.000002 13.587560
48.305595 ; **Au** -0.000001 15.310375 50.742023 ; **Au** 0.000000 17.033183 53.179342

Density matrices

We obtain the self-consistent density on localized numerical orbitals using a 300 Rydberg cut-off and a 0.05eV electronic smearing. Convergence of the density matrices is 10^{-5} . We obtain the self-consistent steady-state density matrix from DFT-PBE as described in Choi, H. J., Cohen, M. L.; Louie, S. G. *Physical Review B*, **2007**, 76, 155420, and Neaton, J. B.; Khoo, K. H.; Spataru, C. D.; Louie, S. G. *Comp. Phys. Comm.*, **2005**, 169, 1, using an $8 \times 8 k_{\parallel}$ -mesh and in a manner equivalent to other work (Brandbyge, M.; Mozos, J. L.; Ordejon, P.; Taylor, J.; Stokbro, K. *Physical Review B*, **2002**, 65, 165401; Xue, Y.; Datta, S.; Ratner, M. A. *Chemical Physics*, **2002**, 281, 151-170; Palacios, J. J.; Pérez-Jiménez, A. J.; Louis, E.; SanFabián, E.; Vergés, J. A. *Physical Review Letters*, **2003**, 90, 106801; Rungger, I.; Sanvito, S. *Physical Review B*, **2008**, 78, 035407). For finite bias calculations –referred to as DFT(V) in the next, the density matrix includes a real axis integration of the scattering-states in the bias window on an adaptive energy grid (Choi, H. J., Cohen, M. L.; Louie, S. G. *Physical Review B*, **2007**, 76, 155420) with a resolution of up to 10^{-7} eV in the vicinity of the molecular resonances.

All the junctions are found to be in the linear response regime, as evidenced by the weak variation of the isocontours of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$.

0-bias and Finite-Bias Transmission Functions

The transmission function is calculated using a $16 \times 16k_{//}$ -mesh, and an energy grid of 100 points between $E_F - 5\text{eV}$ and $E_F + 5\text{eV}$, and 100 supplementary points between $E_F - 50\text{meV}$ and $E_F + 50\text{meV}$. The currents $I(V)$ are calculated through numerical integration of the transmission function $\mathcal{T}(\omega, V)$ in the bias window $E_F - \frac{V}{2}$ and $E_F + \frac{V}{2}$.

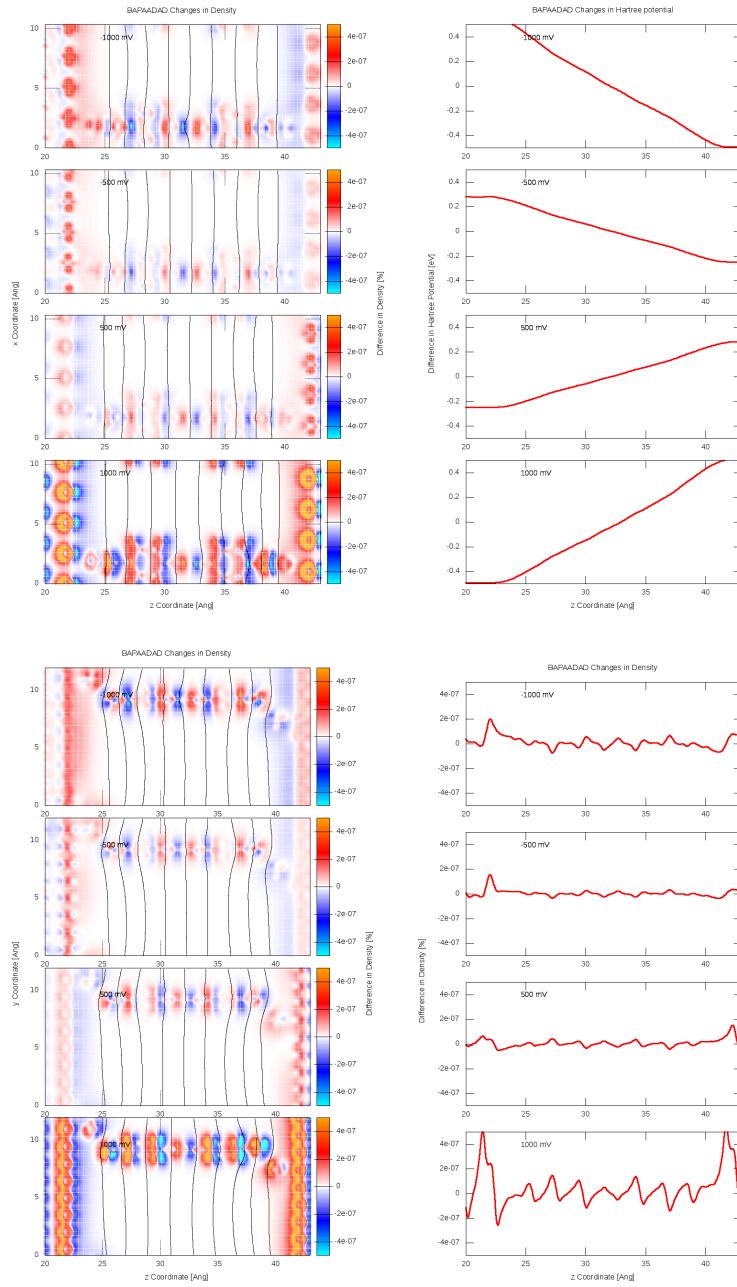


Figure 1: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the APA molecule bonded to two ad-atoms($z \simeq 24\text{\AA}$ and $z \simeq 40\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

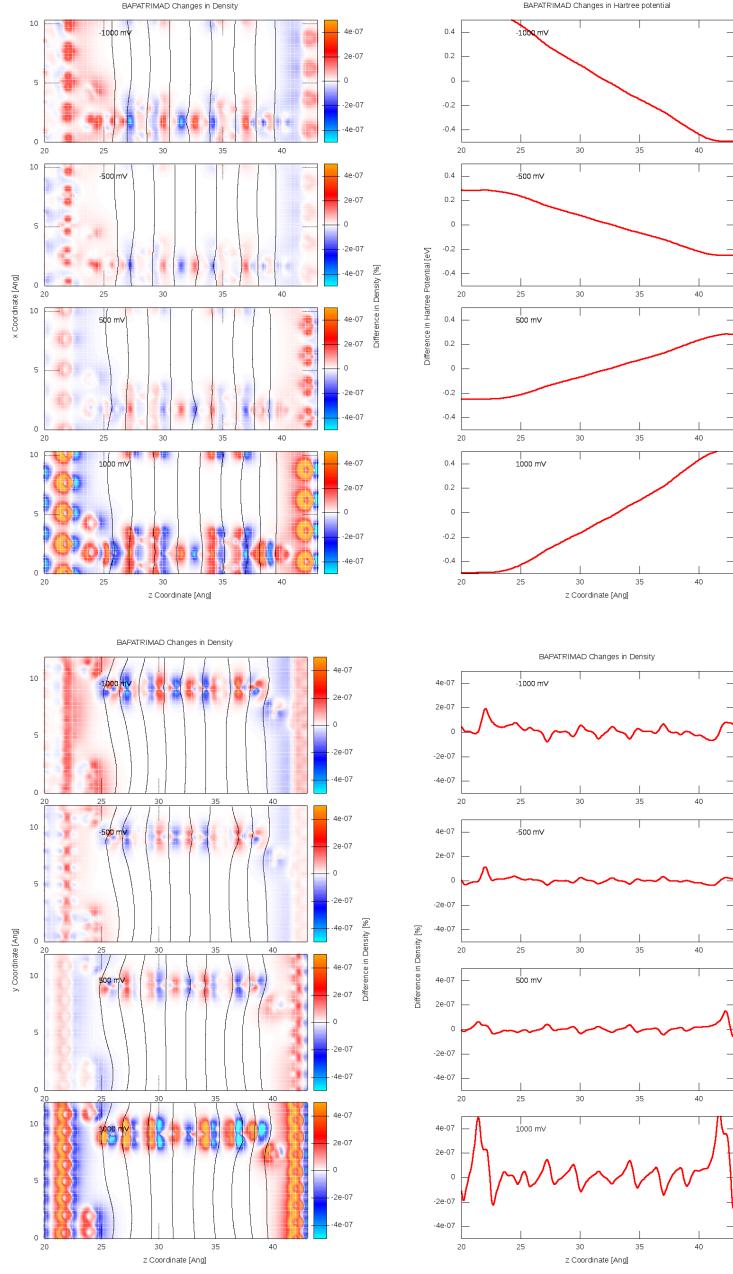


Figure 2: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the APA molecule bonded to one trimer ($z \simeq 24\text{\AA}$) and one ad-atom ($z \simeq 40\text{\AA}$). The contours represent the isovalue of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots +50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x,z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y,z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

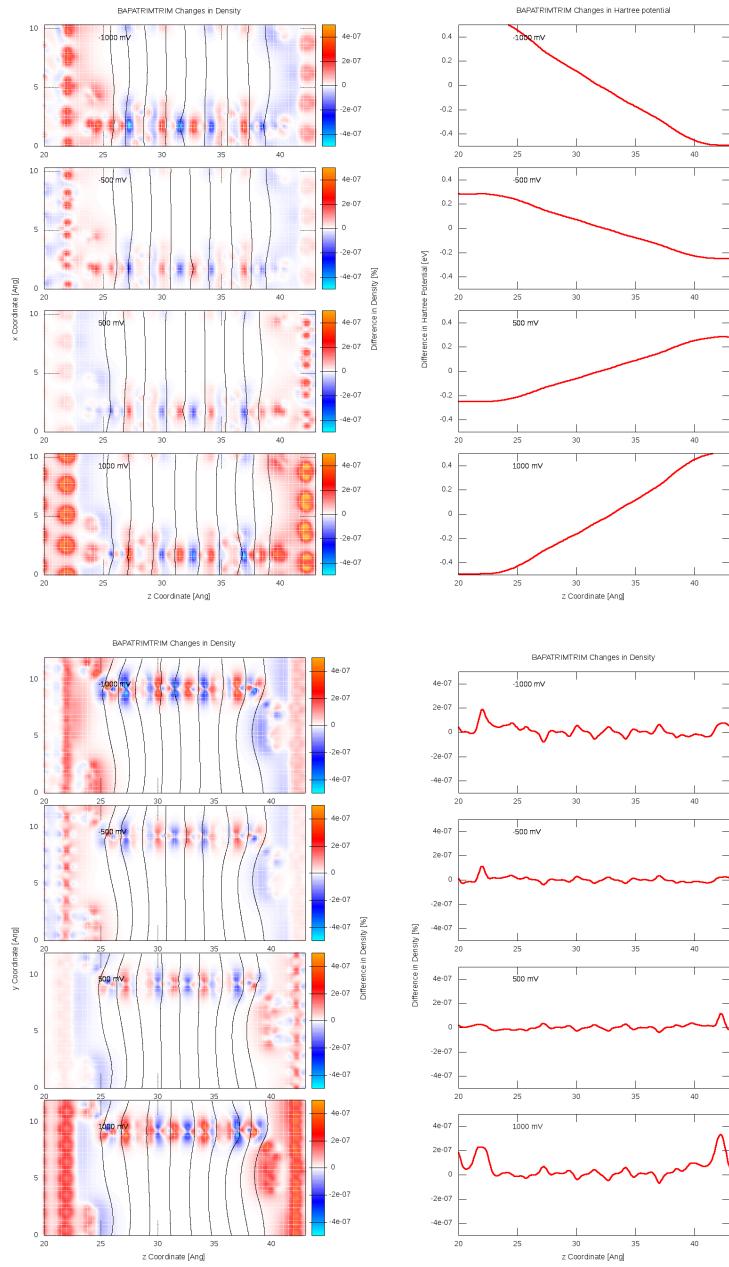


Figure 3: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the APA molecule bonded to two trimers($z \simeq 24\text{\AA}$ and $z \simeq 40\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

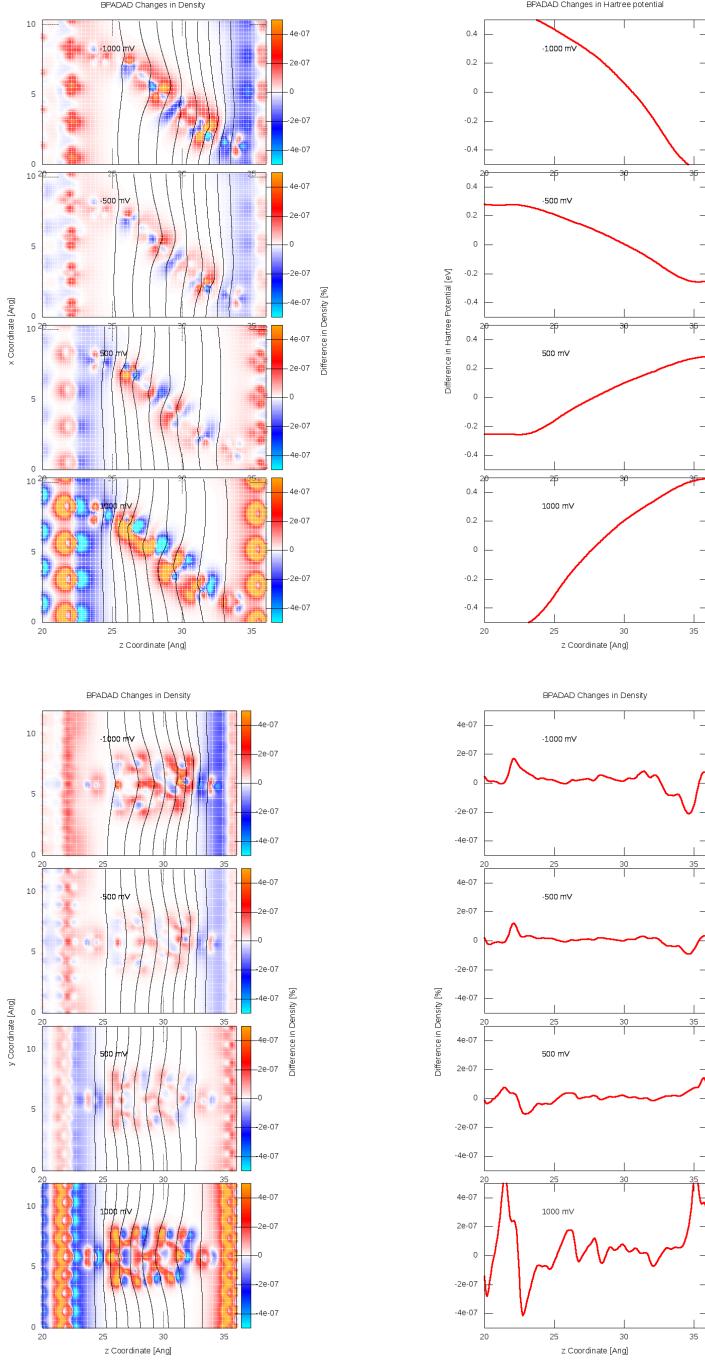


Figure 4: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the BP molecule bonded to two ad-atoms($z \simeq 24\text{\AA}$ and $z \simeq 34\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

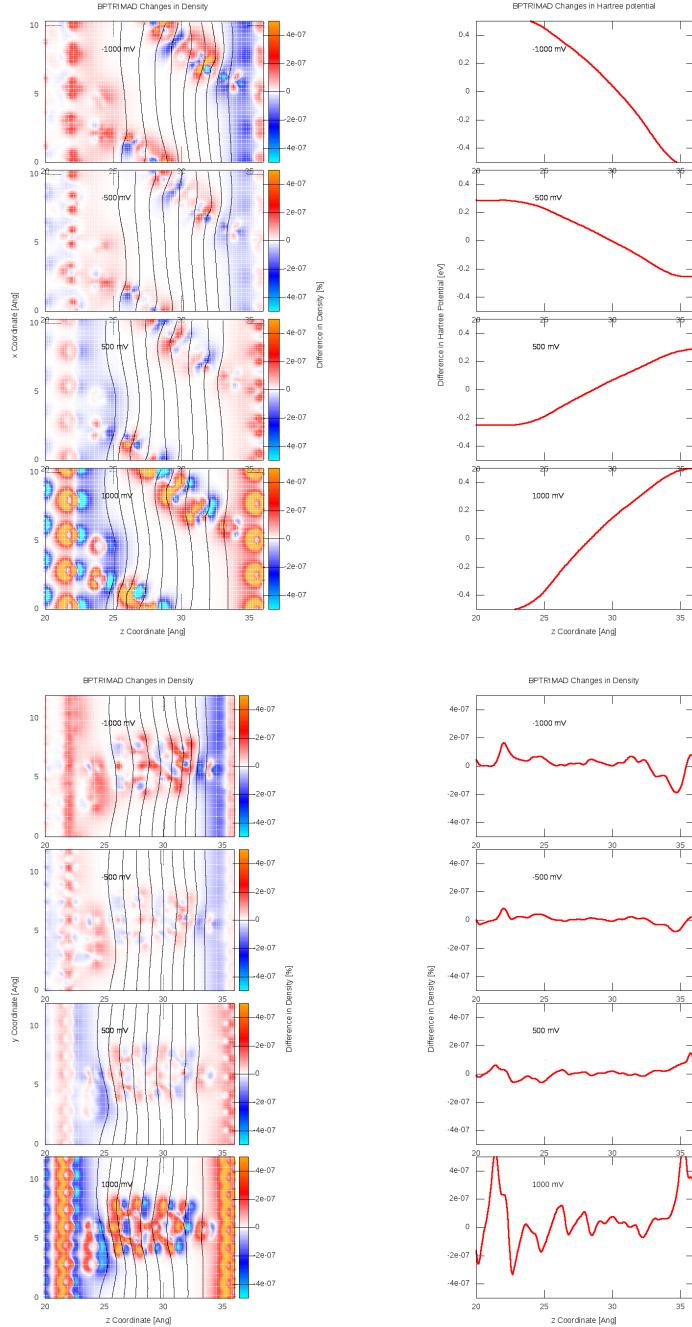


Figure 5: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the BP molecule bonded to one trimer ($z \simeq 24\text{\AA}$) and one ad-atom ($z \simeq 34\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots +50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x,z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y,z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

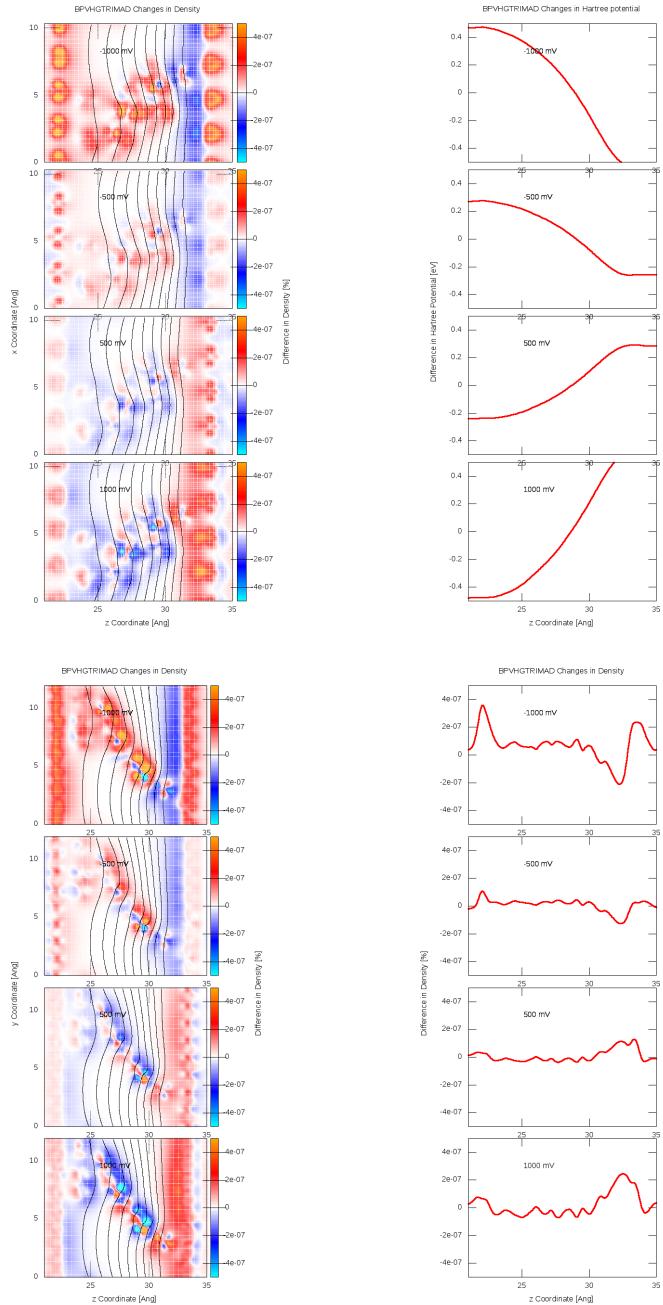


Figure 6: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the BP molecule bonded to one trimer ($z \simeq 24\text{\AA}$) and one ad-atom ($z \simeq 31\text{\AA}$) in the asymmetric geometry for Linear Stark correction. The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

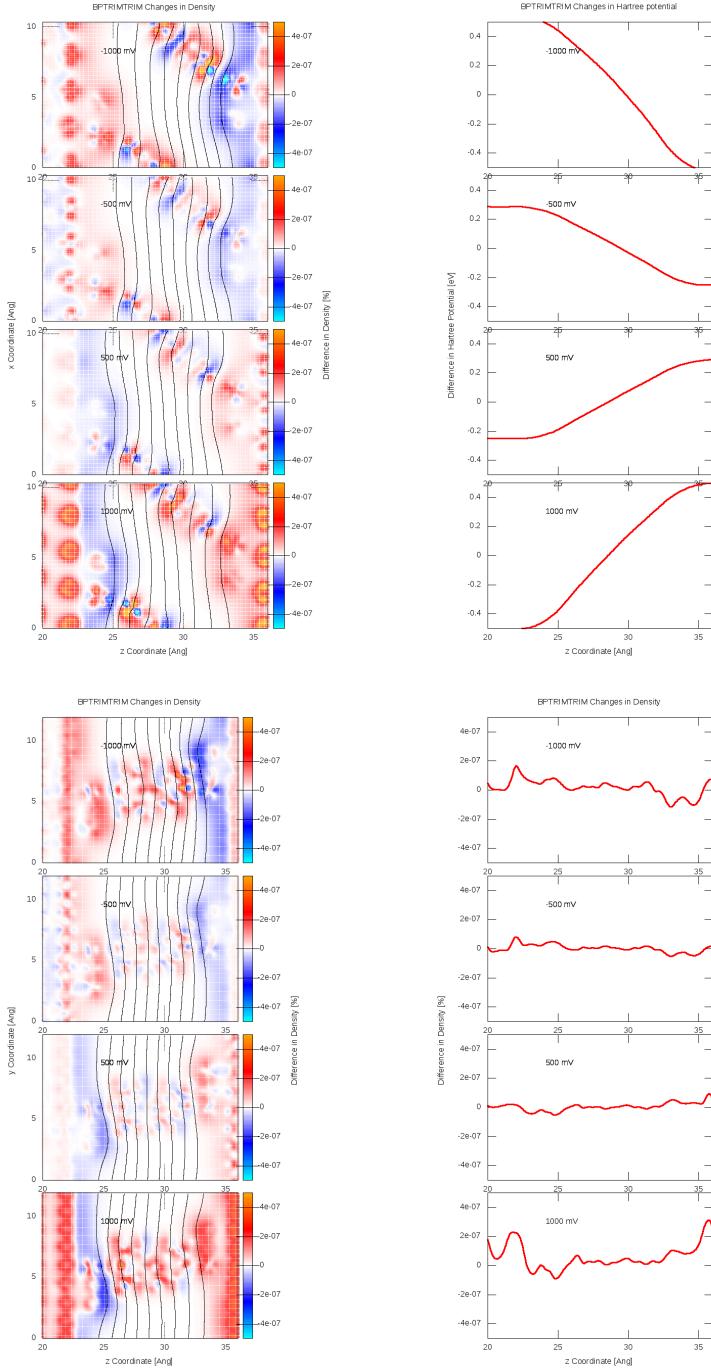


Figure 7: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the BP molecule bonded to two trimers ($z \simeq 24\text{\AA}$ and $z \simeq 34\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

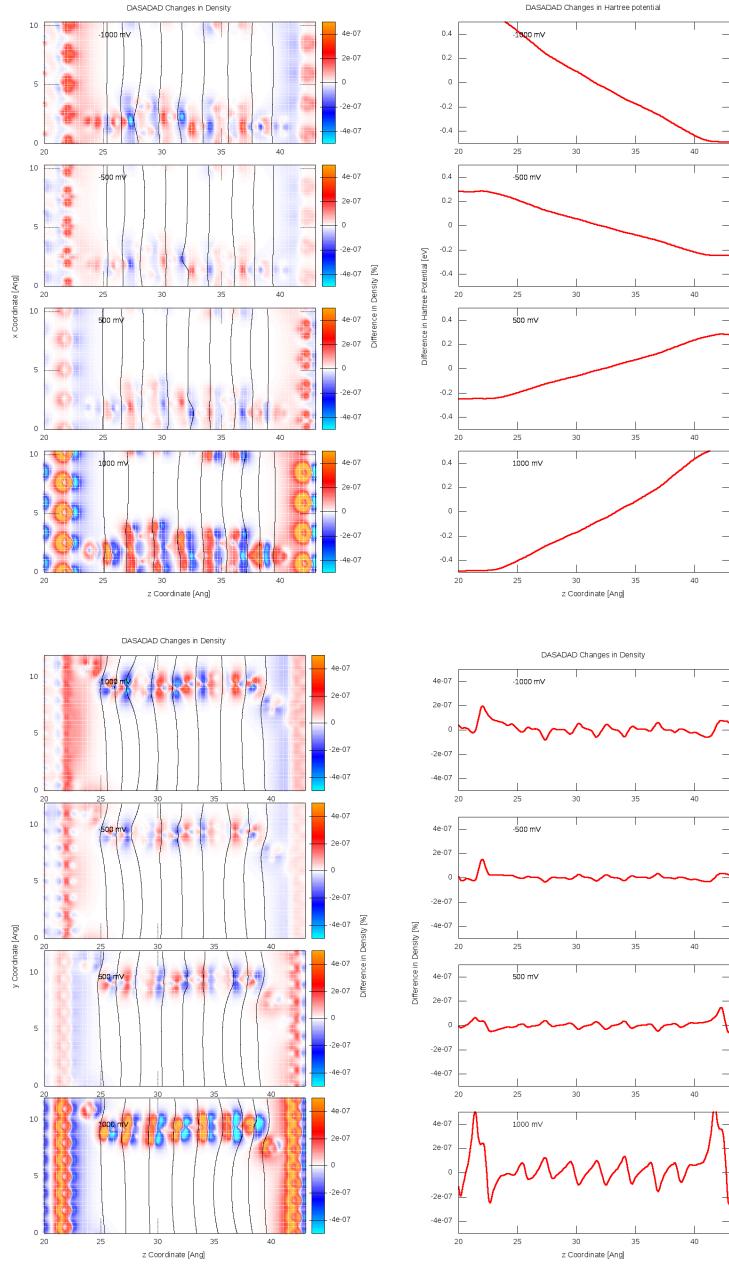


Figure 8: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the DAS molecule bonded to two ad-atoms ($z \simeq 24\text{\AA}$ and $z \simeq 41\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x,z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y,z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

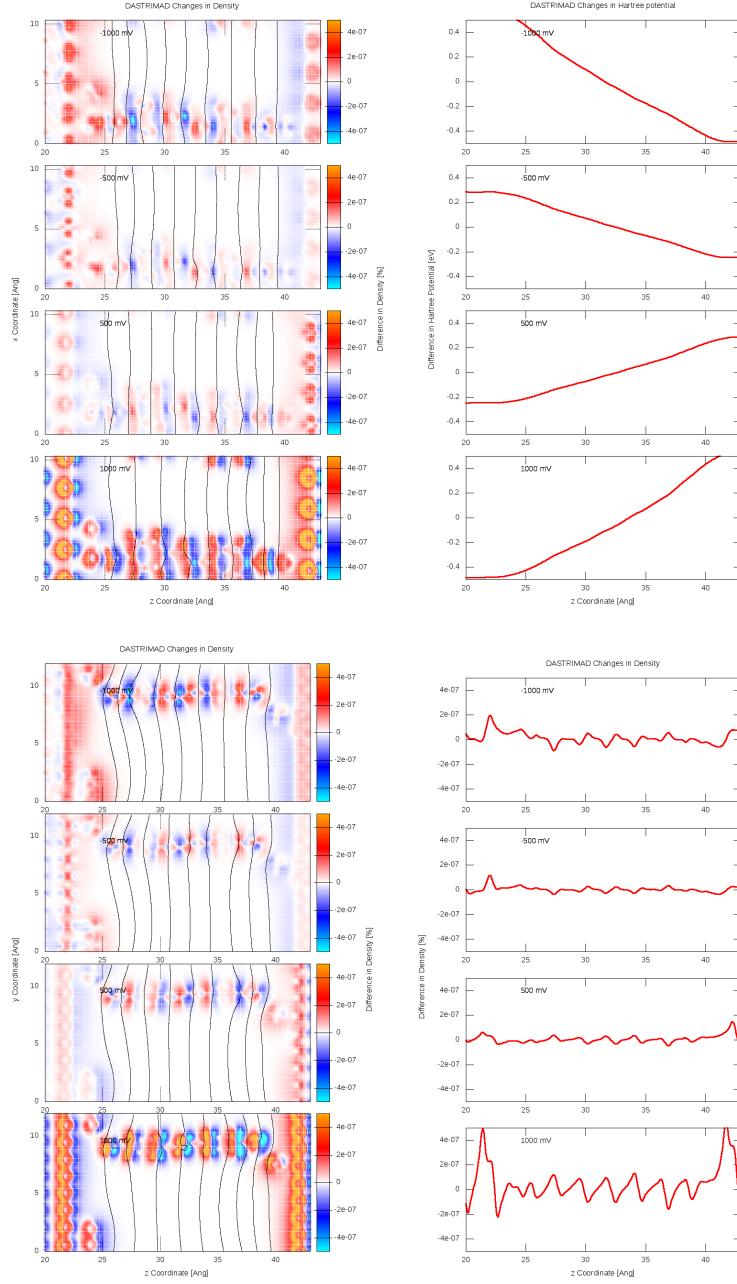


Figure 9: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the DAS molecule bonded to one trimer ($z \simeq 24\text{\AA}$) and one ad-atom ($z \simeq 41\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots +50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x,z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y,z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

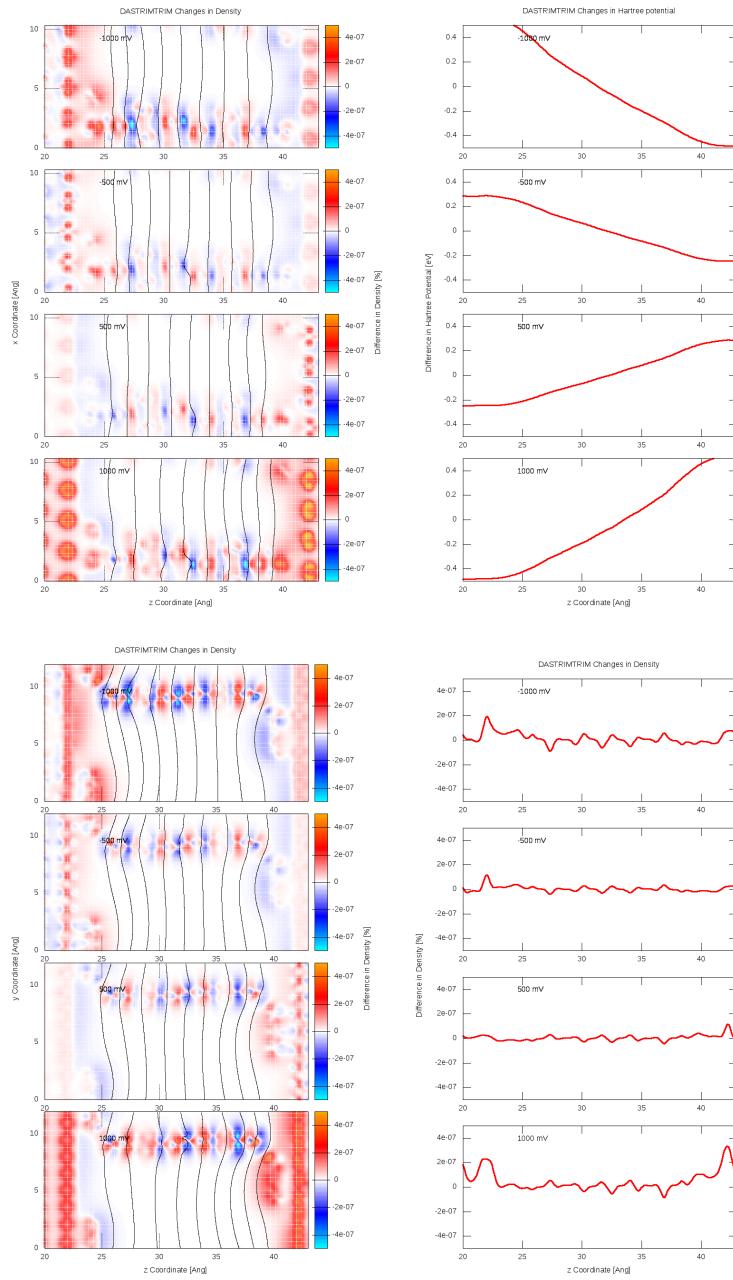


Figure 10: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the DAS molecule bonded to two trimers ($z \simeq 24\text{\AA}$ and $z \simeq 41\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

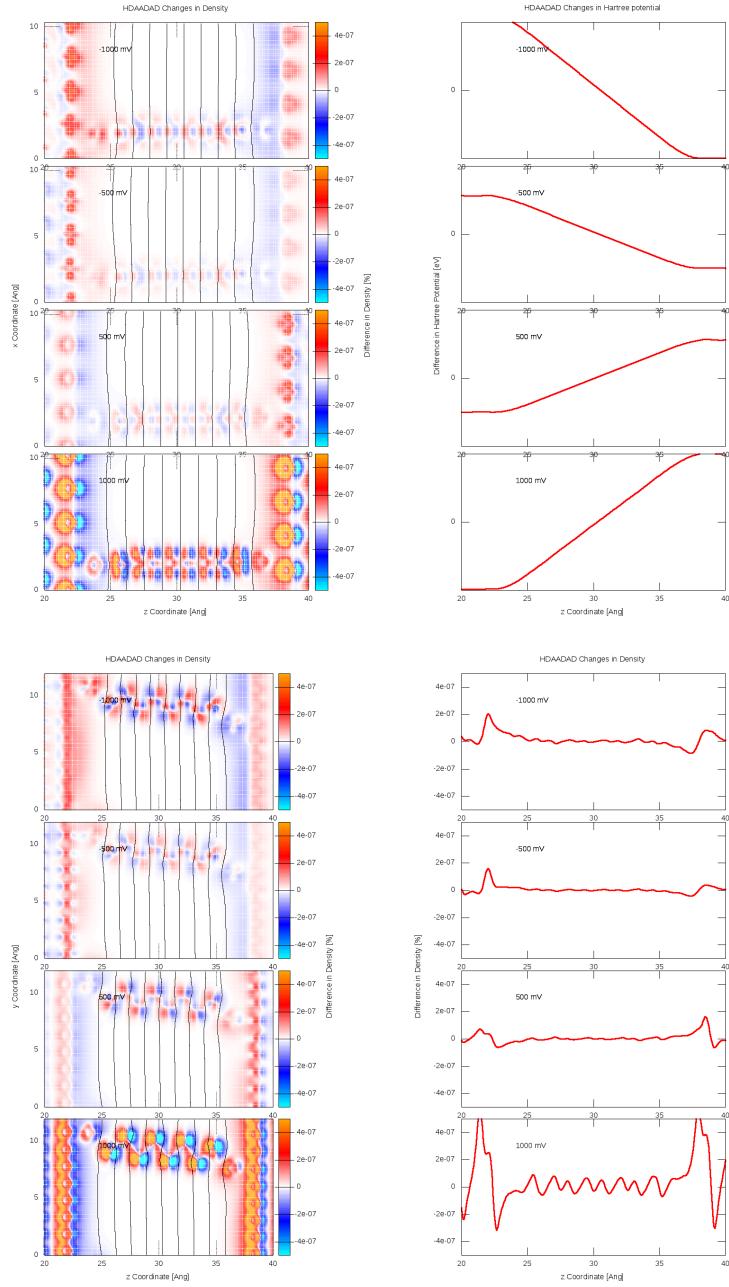


Figure 11: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the HDA molecule bonded to two ad-atoms ($z \simeq 24\text{\AA}$ and $z \simeq 37\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x, z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y, z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

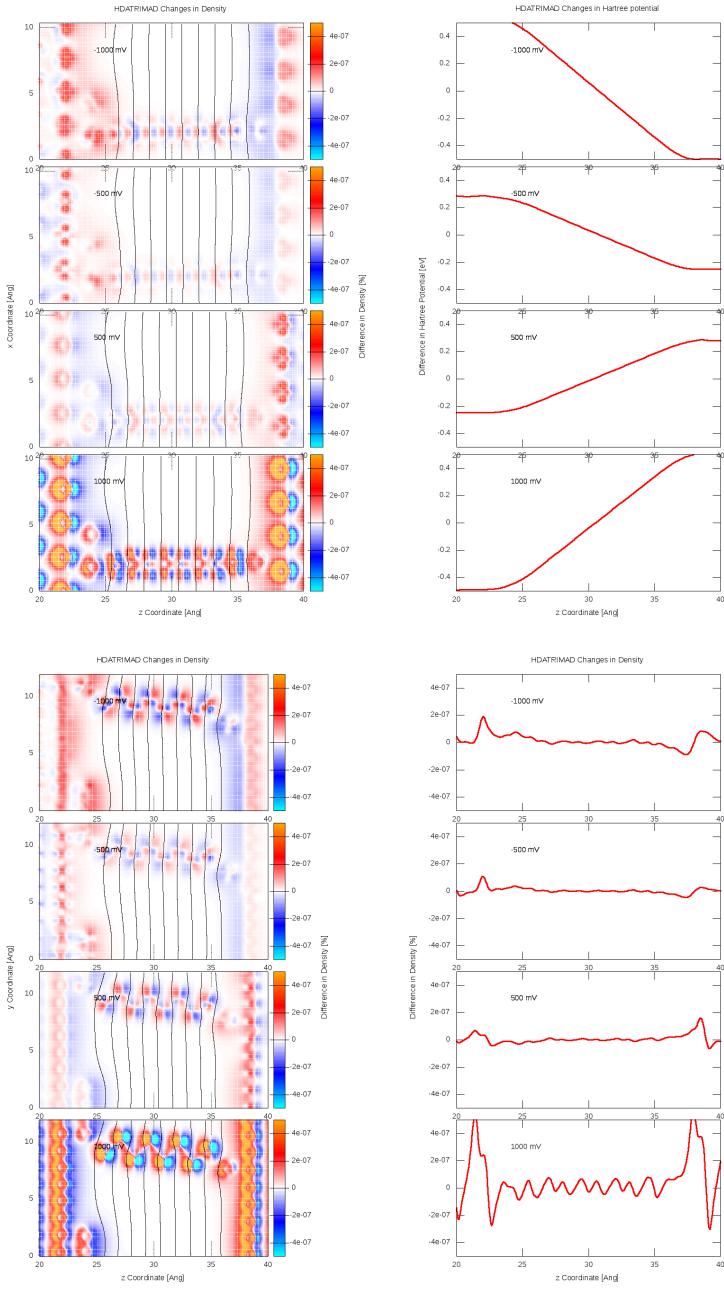


Figure 12: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the HDA molecule bonded to one trimer ($z \approx 24\text{\AA}$) and one ad-atom ($z \approx 37\text{\AA}$). The contours represent the isovalues of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x,z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y,z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

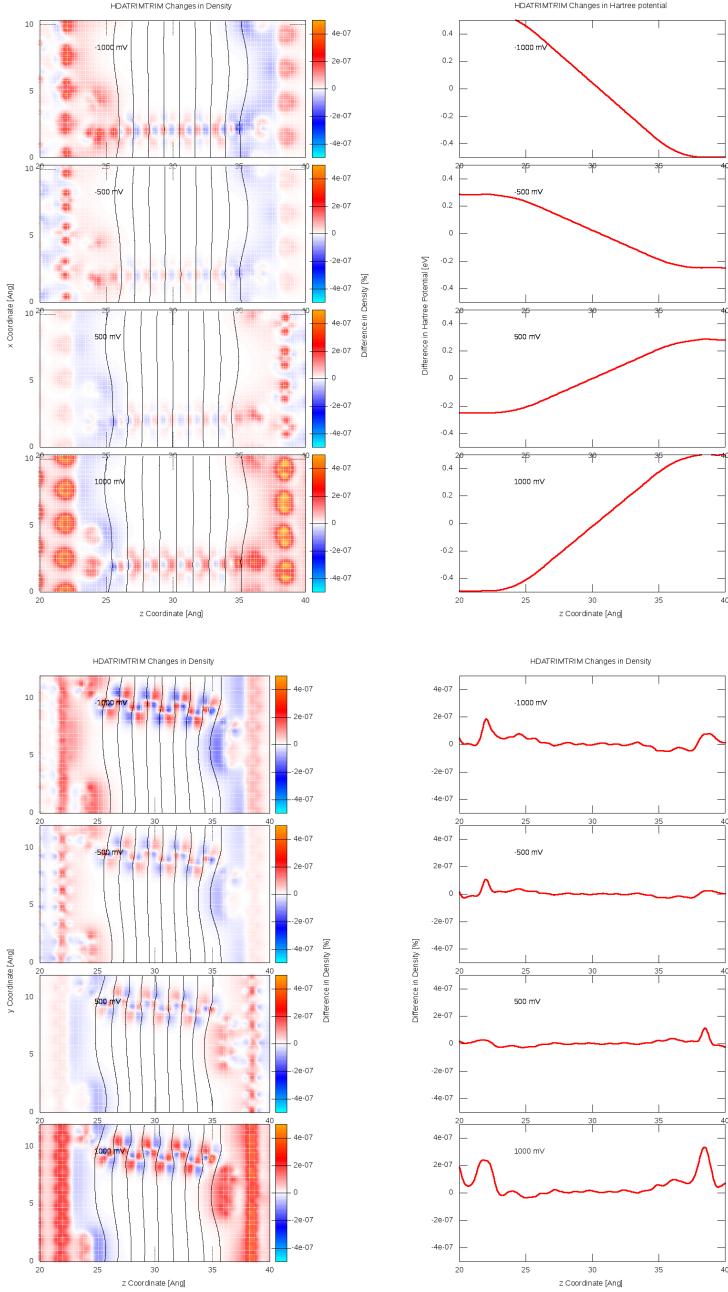


Figure 13: DFT-PBE differences in density and Hartree potentials for biases going from -1000mV to 1000mV relative to their zero-bias values for the HDA molecule bonded to two trimers ($z \simeq 24\text{\AA}$ and $z \simeq 37\text{\AA}$). The contours represent the isovalue of the Hartree potential scaled by the applied bias $\frac{\Delta U_H}{V} = -50\%, -40\% \dots + 50\%$. Top Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (x,z) planes. Bottom Left: Average changes in the self-consistent DFT-PBE(V) density matrix and Hartree potential in the (y,z) planes. Top Right: Average changes in the self-consistent DFT-PBE(V) Hartree potential along the z -axis. Bottom Right: Average changes in the self-consistent DFT-PBE(V) Density along the z -axis.

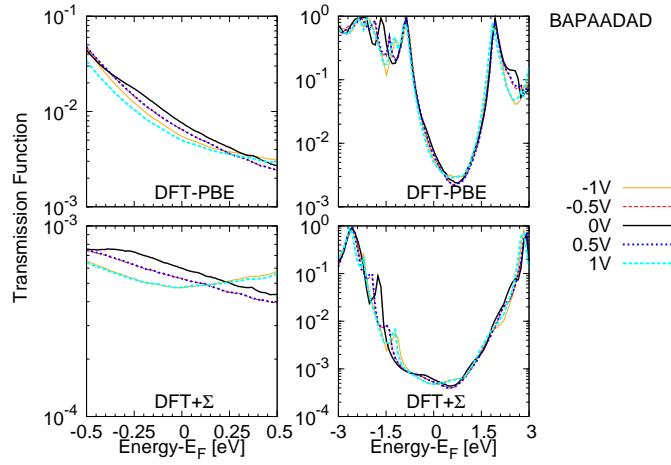


Figure 14: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the APA molecule bonded to two adatoms. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

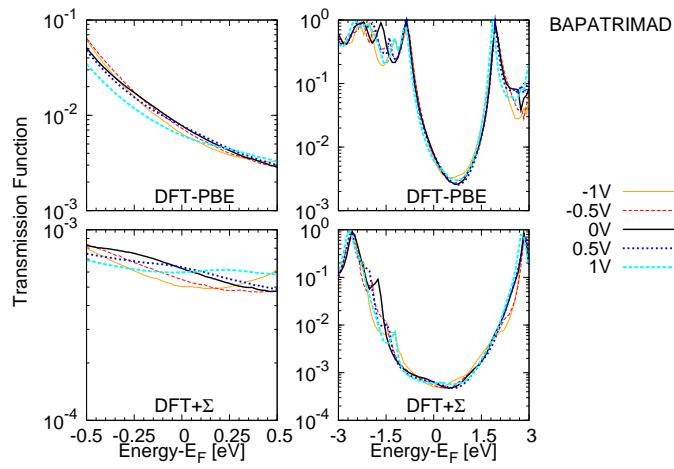


Figure 15: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the APA molecule bonded to one trimer and one adatom. Left: Maximal bias window $[E_F - 0.5eV; E_F + 0.5eV]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3eV; E_F + 3eV]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

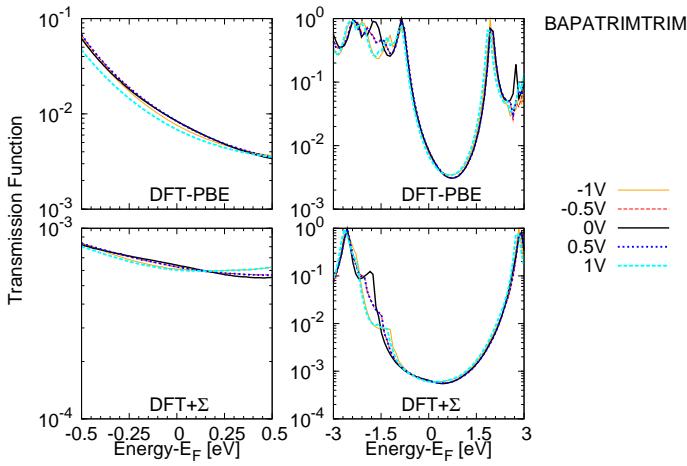


Figure 16: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the APA molecule bonded to two trimers. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

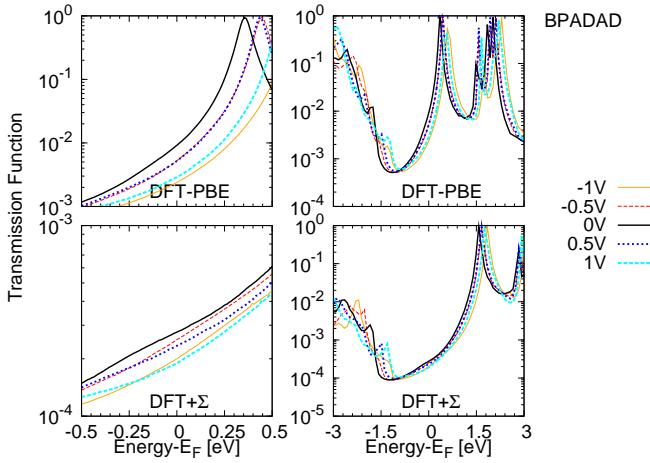


Figure 17: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the BP molecule bonded to two adatoms. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

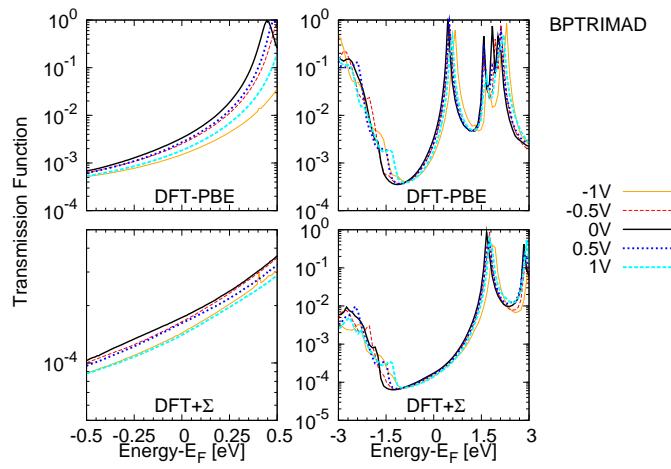


Figure 18: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the BP molecule bonded to one trimer and one adatom. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

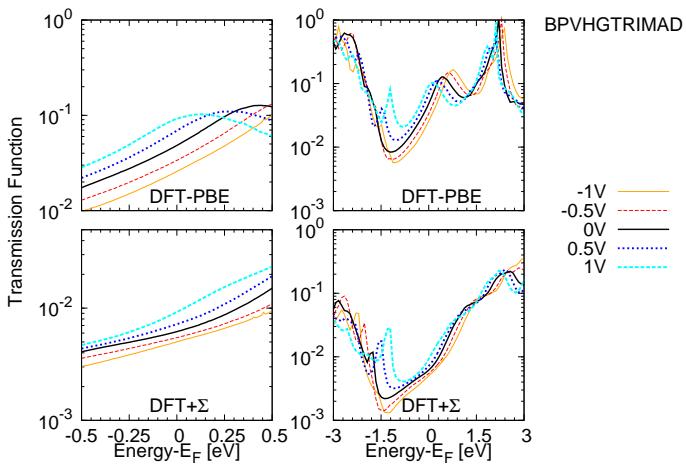


Figure 19: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the BP molecule bonded to one trimer and one adatom, in the geometry used for the Linear Stark correction calculation. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

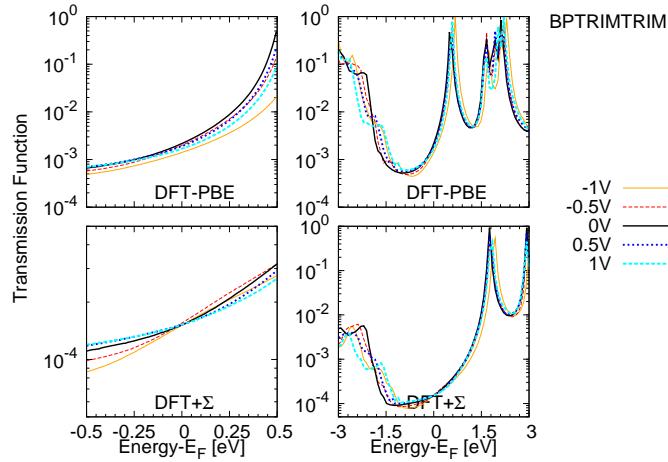


Figure 20: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the BP molecule bonded to two trimers. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

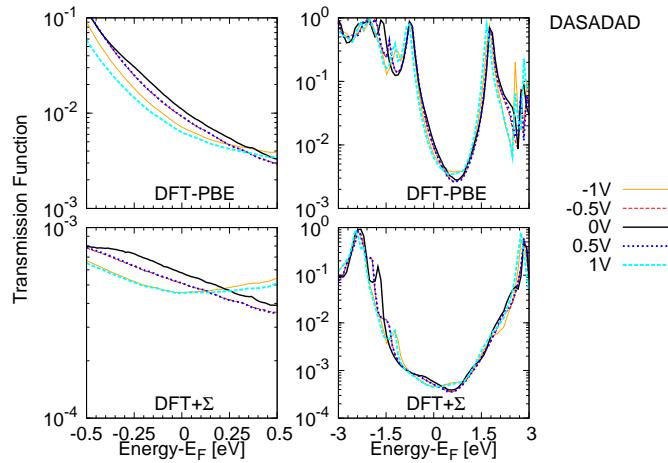


Figure 21: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the DAS molecule bonded to two adatoms. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

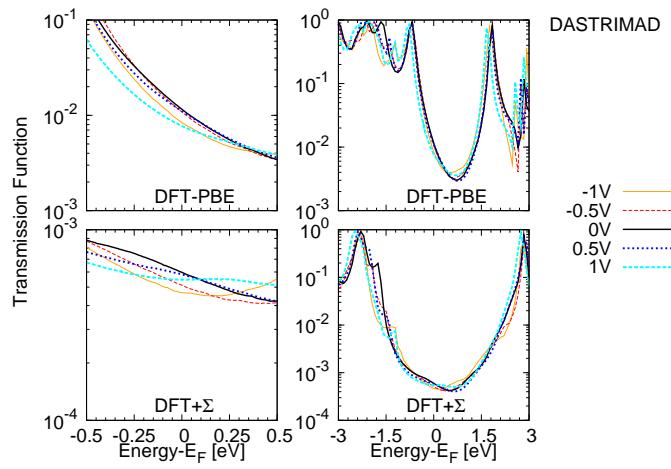


Figure 22: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the DAS molecule bonded to one trimer and one adatom. Left: Maximal bias window $[E_F - 0.5eV; E_F + 0.5eV]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3eV; E_F + 3eV]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

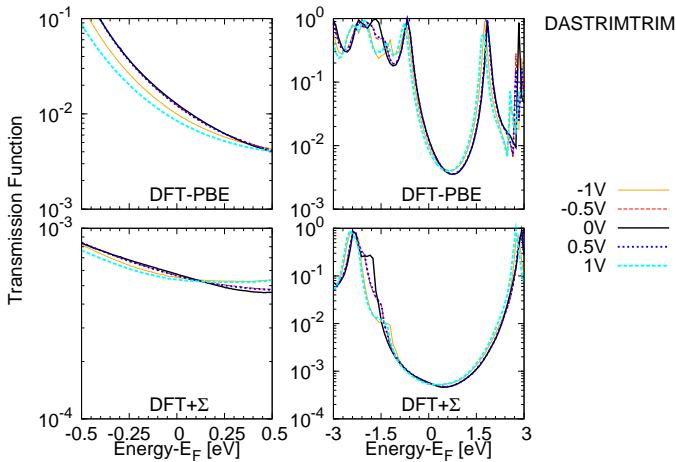


Figure 23: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the DAS molecule bonded to two trimers. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

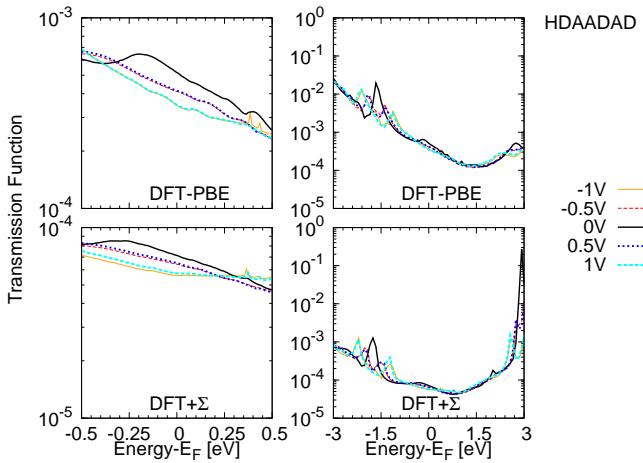


Figure 24: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the HDA molecule bonded to two adatoms. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

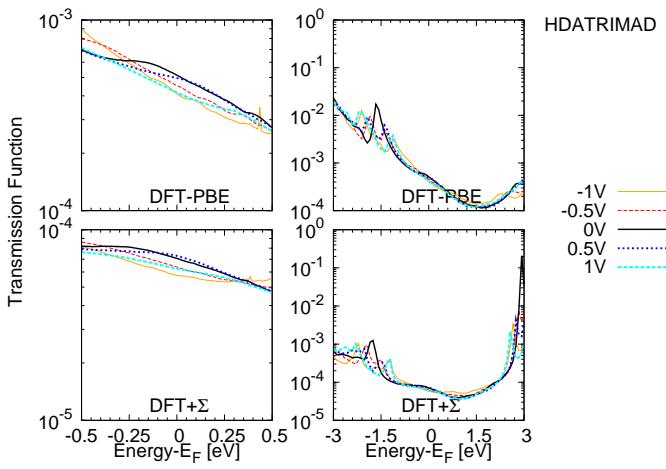


Figure 25: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the HDA molecule bonded to one trimer and one adatom. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.

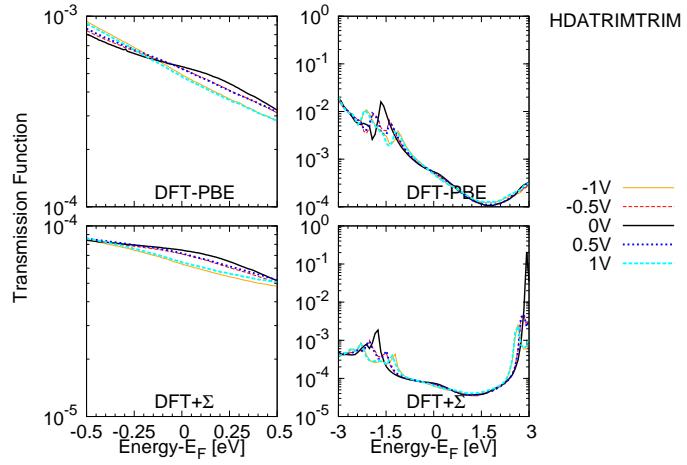


Figure 26: Transmission functions for biases going from $-1000mV$ to $1000mV$ for the HDA molecule bonded to two trimers. Left: Maximal bias window $[E_F - 0.5\text{eV}; E_F + 0.5\text{eV}]$ where E_F is the average Fermi energy of the system; Right: $[E_F - 3\text{eV}; E_F + 3\text{eV}]$ window; Top: Transmission functions as calculated from DFT-PBE(V); Bottom: Transmission functions calculated with DFT(V)+ Σ . The currents reported in Fig. 1 are calculated as the integral between $[E_F - \frac{V}{2}; E_F + \frac{V}{2}]$ of the transmission function for a given bias V , multiplied by $\frac{2e}{h}$.