

Adequacy of Si:P Chains as Fermi-Hubbard Simulators: Supplemental Material

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HAMILTONIAN PARAMETERS

We extend the single particle parametrization presented in Ref. [1] to include corrections up to nearest neighbors potentials and calculate electron-electron interactions (U and V) including effects of screening of the crystal environment. The coulomb potential considered (Eq. 4) is presented in Ref. [2] and briefly discussed in section ENVELOPE INTEGRALS.

We begin with an atomistic Hamiltonian consisting of kinetic energy \hat{K} and all core potentials $\sum_n \hat{V}_n$. Given that we are interested in the matrix elements $\langle j|\hat{H}|i\rangle$, we are going to exploit its functional form and rewrite it as $\hat{H} = \hat{H}_i + \hat{H}'$ with the single donor hamiltonian $\hat{H}_i = \hat{K} + \hat{V}_i$ consisting in kinetic energy and core potential for the i donor and \hat{H}' the perturbation potential due to all other cores. This arrangement of terms is very useful since we are spanning the Hilbert space with donor (dopant) orbitals, $\hat{H}_i|i\rangle = -E_0|i\rangle$ where E_0 is the single donor binding energy. We are going to consider \hat{H}_i and restrict \hat{H}' contribution to nearest neighbor donors neglecting all other terms—this is an extension of the procedure described in Ref. [1]. Given this, the expression for the hopping will be,

$$t_{ij} = \langle j|\hat{H}_i|i\rangle + \langle j|\hat{H}'|i\rangle \quad (1a)$$

$$\approx -E_0 S(\mathbf{R}) + \langle j|\hat{V}_j|i\rangle \quad (1b)$$

$$= \mathcal{T}_{ij}(R)\Theta_v(\mathbf{R}) \quad (1c)$$

$$\Theta_v = \frac{1}{3} [\cos(k_0 R_x) + \cos(k_0 R_y) + \cos(k_0 R_z)] \quad (1d)$$

where, $R = |\mathbf{R}| = |\mathbf{R}_{ij}|$ is the interdonor distance. The hopping t_{ij} will be a function of E_0 , the overlap of orbitals i and j , $S(\mathbf{R}) = \langle j|i\rangle$, and a correction due to the core potential of j . Solving each term the final expression will be the product of the oscillatory part Θ_v and a sum of envelopes integrals, \mathcal{T}_{ij} .

In a similar way, the onsite energy expression,

$$\varepsilon_i = \langle i|\hat{H}_i|i\rangle + \langle i|\hat{H}'|i\rangle \approx -E_0 + \sum_{j=i\pm 1} \mathcal{E}_j, \quad (2)$$

contemplates E_0 , and corrections due to the two nearest neighbors core potential a function of envelopes only, \mathcal{E}_j .

Electron-electron terms are calculated by the formal definition,

$$V_{ijkl} = \int d^3r_1 \int d^3r_2 \Psi_i^*(\mathbf{r}_1) \Psi_j^*(\mathbf{r}_2) V(\mathbf{r}_{21}) \Psi_k(\mathbf{r}_2) \Psi_l(\mathbf{r}_1), \quad (3)$$

but the model is restricted to $V_{iiii} = U$ (Hubbard) and $V_{jiii} = V$ (Direct), the dominant terms. All integrals are defined only by the envelopes.

All terms, \mathcal{E}_j , \mathcal{T}_{ij} , U and V , are presented in section ENVELOPE INTEGRALS.

ENVELOPE INTEGRALS

We consider in this work a complete potential, among electron-electron and electron-core, incorporating screening,

$$V(r) = \pm \frac{e^2}{4\pi r} \left(\frac{1}{\epsilon_{Si}} + \frac{1}{\epsilon^*} e^{-r/r^*} \right), \quad (4)$$

where $1/\epsilon^* = (1/\epsilon_0 - 1/\epsilon_{Si})$, ϵ_{Si} (ϵ_0) Si (vacuum) static dielectric constant respectively, and r^* is the screening constant. This potential consists in two parts, (a) a standard bare point charge ($\propto \frac{1}{r}$) part and (b) a screened point

charge term ($\propto \frac{e^{-r/r^*}}{r}$). All results presented here hold for envelopes as defined in the main text, i.e., for an electron 1, pinned to a donor A with position vectors \mathbf{r}_1 and \mathbf{R}_A respectively, $F(r_{1,A}) = (\pi a^*{}^3)^{-1/2} \exp(-r_{1,A}/a^*)$ where $r_{1,A} = |\mathbf{r}_1 - \mathbf{R}_A|$ as the electron 1 relative position to donor A . Coordinates \mathbf{R}_A and \mathbf{R}_B correspond to donors A and B , and \mathbf{r}_1 and \mathbf{r}_2 to electrons 1 and 2, respectively. $R = |\mathbf{R}_B - \mathbf{R}_A|$ is the interdonor and $r_{12} = |\mathbf{r}_2 - \mathbf{r}_1|$ the interelectron distances. We make use of convenient set of dimensionless constants: $w = R/a^*$, $m = R/2r^*$, $w_+ = (w + m)$, $w_- = (w - m)$, making expressions more compact.

The bare point charge and overlap integrals can be easily performed with a convenient change to prolate spheroidal coordinates—or spherical coordinates if applicable [3–5],

$$\begin{aligned} S_{AB} &= \langle F(r_{1,B}) | F(r_{1,A}) \rangle = \left(1 + w + \frac{w^2}{3}\right) e^{-w} \\ I_{AA} &= \langle F(r_{1,A}) | \frac{1}{r_{1,B}} | F(r_{1,A}) \rangle = \frac{1}{R} [1 - (1 + w) e^{-2w}] \\ I_{AB} &= \langle F(r_{1,B}) | \frac{1}{r_{1,B}} | F(r_{1,A}) \rangle = \frac{1}{R} (w + w^2) e^{-w} \\ I_{AAAA} &= \langle F(r_{2,A}) F(r_{1,A}) | \frac{1}{r_{12}} | F(r_{1,A}) F(r_{2,A}) \rangle = \frac{1}{a_{sc}} \frac{5}{8} \\ I_{ABBA} &= \langle F(r_{2,A}) F(r_{1,B}) | \frac{1}{r_{12}} | F(r_{1,B}) F(r_{2,A}) \rangle = \frac{1}{R} \left[1 - \left(1 + \frac{11}{8}w + \frac{3}{4}w^2 + \frac{1}{6}w^3\right) e^{-2w}\right] \end{aligned}$$

Although the same change of coordinates make equivalent integrals with a screened potential performable, an increase in complexity make these integrals not so straightforward neither easily found in literature, results are presented below,

$$\begin{aligned} I_{AA}^* &= \langle F(r_{1,A}) | \frac{e^{-r_{1,B}/r^*}}{r_{1,B}} | F(r_{1,A}) \rangle = \frac{1}{R} \frac{w^3}{w_+^2 w_-^2} [w e^{-2m} - (w + w^2 - m^2) e^{-2w}] \\ I_{AB}^* &= \langle F(r_{1,B}) | \frac{e^{-r_{1,B}/r^*}}{r_{1,B}} | F(r_{1,A}) \rangle = \frac{1}{R} \frac{w^3}{w_+^2} e^{-w} \left[1 + \frac{w}{m} + \frac{w}{2m^2} (e^{-2m} - 1)\right] \\ I_{AAAA}^* &= \langle F(r_{2,A}) F(r_{1,A}) | \frac{e^{-r_{12}/r^*}}{r_{12}} | F(r_{1,A}) F(r_{2,A}) \rangle = \frac{1}{a_{sc}} \frac{1}{k_+^2 k_-^2} \left(\frac{k_+ k_-}{2} - 4 + \frac{64}{k_+^2}\right) \\ I_{ABBA}^* &= \langle F(r_{2,A}) F(r_{1,B}) | \frac{e^{-r_{12}/r^*}}{r_{12}} | F(r_{1,B}) F(r_{2,A}) \rangle = \frac{1}{R} \frac{w^3}{24w_+^4 w_-^4} (24w^5 e^{-2m} + P_d e^{-2w}) \end{aligned}$$

here P_d is a polynomial of w and m (as shown below). To highlight that the Hubbard integrals (for a given a^* and r^* parameters) does not depend on R , we express it as a function of $k_{\pm} = (a^* \pm 2r^*)/r^*$. In the direct term,

$$P_d = -24w^4(w + w_+ w_-) - w_+^2 w_-^2 [6w^2(1 + 2w) + w_+ w_- (3 + 6w + 4w^2)].$$

HAMILTONIAN PARAMETERS: EXPLICIT EXPRESSIONS

We present expressions for hamiltonian parameters as a function of envelope integrals in this section \mathcal{E}_A (onsite), \mathcal{T}_{AB} (hopping), U_A (Hubbard) and V_{AB} (direct) terms,

$$\begin{aligned} \mathcal{E}_A &= -\frac{e^2}{4\pi\epsilon_{Si}} I_{AA} - \frac{e^2}{4\pi\epsilon_{sc}} I_{AA}^* \\ \mathcal{T}_{AB} &= -E_0 S_{AB} - \frac{e^2}{4\pi\epsilon_{Si}} I_{AB} - \frac{e^2}{4\pi\epsilon_{sc}} I_{AB}^* \\ U_A &= \frac{e^2}{4\pi\epsilon_{Si}} I_{AAAA} + \frac{e^2}{4\pi\epsilon_{sc}} I_{AAAA}^* \\ V_{AB} &= \frac{e^2}{4\pi\epsilon_{Si}} I_{ABBA} + \frac{e^2}{4\pi\epsilon_{sc}} I_{ABBA}^* \end{aligned}$$

where e is the electron charge and E_0 is the single donor binding energy.

EXPLORING ELECTRONIC PHASES BY CHANGES IN INTERDONOR SEPARATION

Different donor-donor distances lead to Hamiltonian parameters that span the phase diagram of spin and charged ordered states, including the bond-order phase. In Fig. 1, we see that for distances 2.69nm up to 3.46nm, the BOW state is achievable.

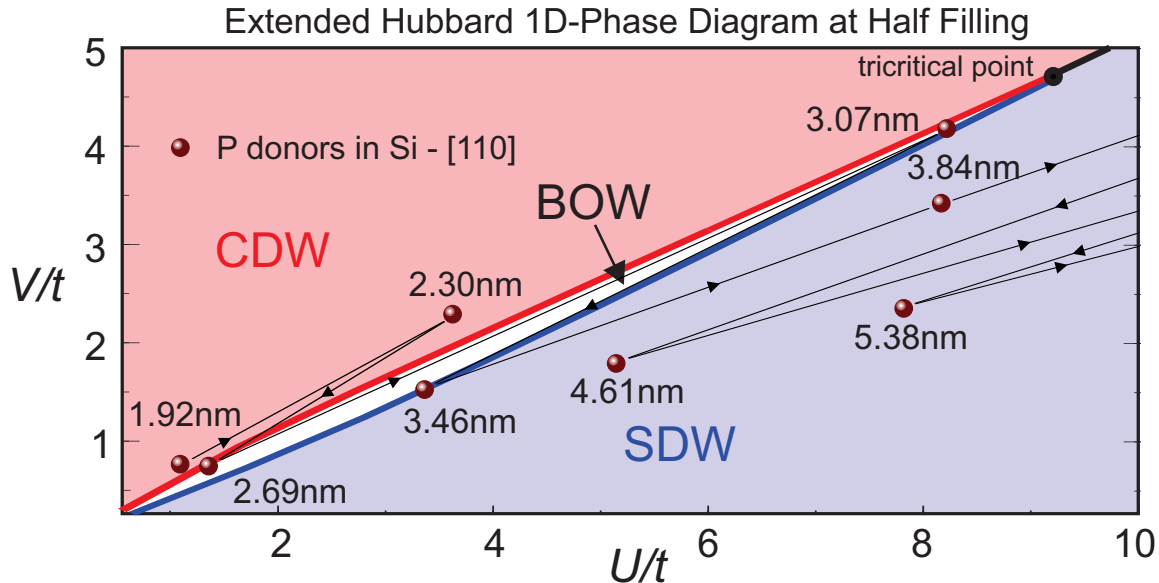


FIG. 1. Extended Hubbard 1D phase diagram at half filling as in Ref. [6]. Spheres show allowed position for P donors in Si along [110] direction. The numbers in nm correspond to interdonor distance R_0 , beginning by $R_0 = 1.92\text{nm}$, with black arrows pointing direction of increasing R_0 .

CORRELATIONS: BEHAVIOR AT EXTREME TEMPERATURES

We present, for comparison, results for C_j (Fig. 2) and S_j (Fig. 3). In all case, no correlation signature can be observed for $T=300\text{K}$. For $T=0$, C_j shows a very short-range correlation relation, while S_j presents correlation length bigger than chain size. The periodic boundary condition, presented in the main text, implies in correlations in site 8 to be equal to correlations in site 2, for example.

CORRELATIONS: BOUNDARY CONDITIONS

Our periodic boundary conditions were chosen for definiteness. We also have simulations with open boundary conditions, which we added to the supplemental material. The obvious consequence is the appearance of chain-end excited states, which account for the minor differences illustrated in S_j results shown in Fig. 4. These results do not change any of our conclusions.

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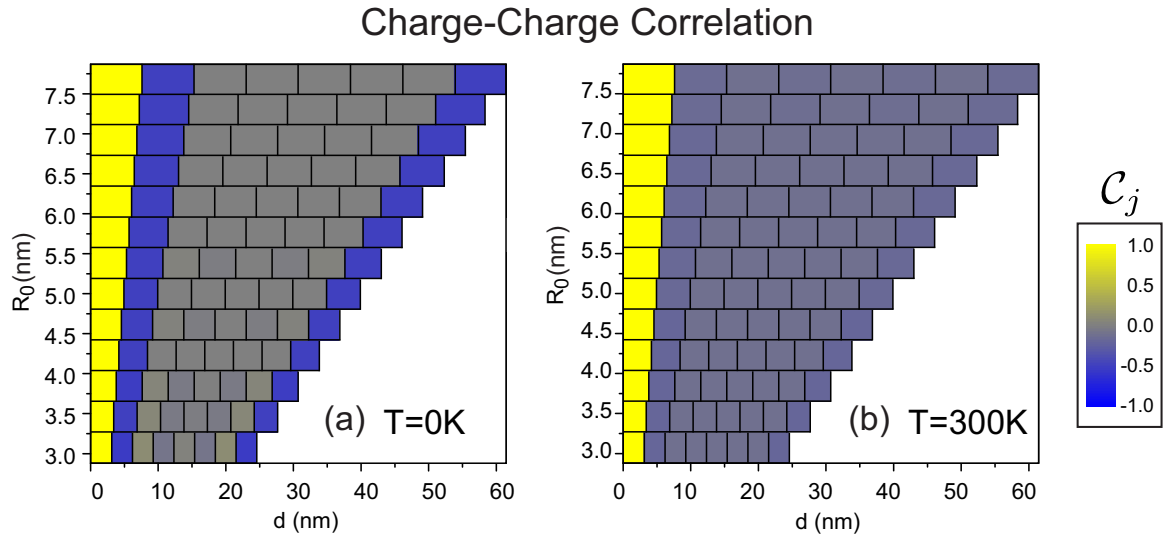


FIG. 2. Calculated charge-charge correlations for extreme temperatures. The low-temperature limit corresponds to $T = 0\text{K}$, while for the high temperature limit we take arbitrarily $T = 300\text{K}$, which is not physical meaningful (see text). Each box shows C_j (see color code) as a function of interdonor distance (R_0) and position along the chain (d). As expected (a) $T=0\text{K}$ shows maximum correlations and (b) $T=300\text{K}$ shows no signature of correlation.

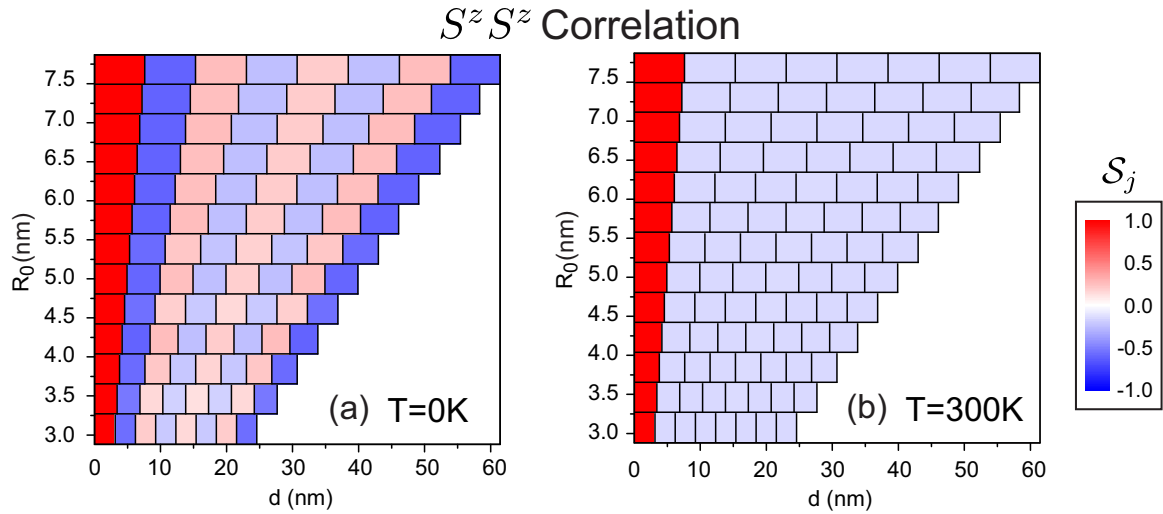


FIG. 3. Calculated $S^z S^z$ correlations for extreme temperatures. The low-temperature limit corresponds to $T = 0\text{K}$, while for the high temperature limit we take arbitrarily $T = 300\text{K}$, which is not physical meaningful (see text). Each box shows S_j (see color code) as a function of interdonor distance (R_0) and position along the chain (d). As expected (a) $T=0\text{K}$ shows maximum correlations and (b) $T=300\text{K}$ shows no signature of correlation.

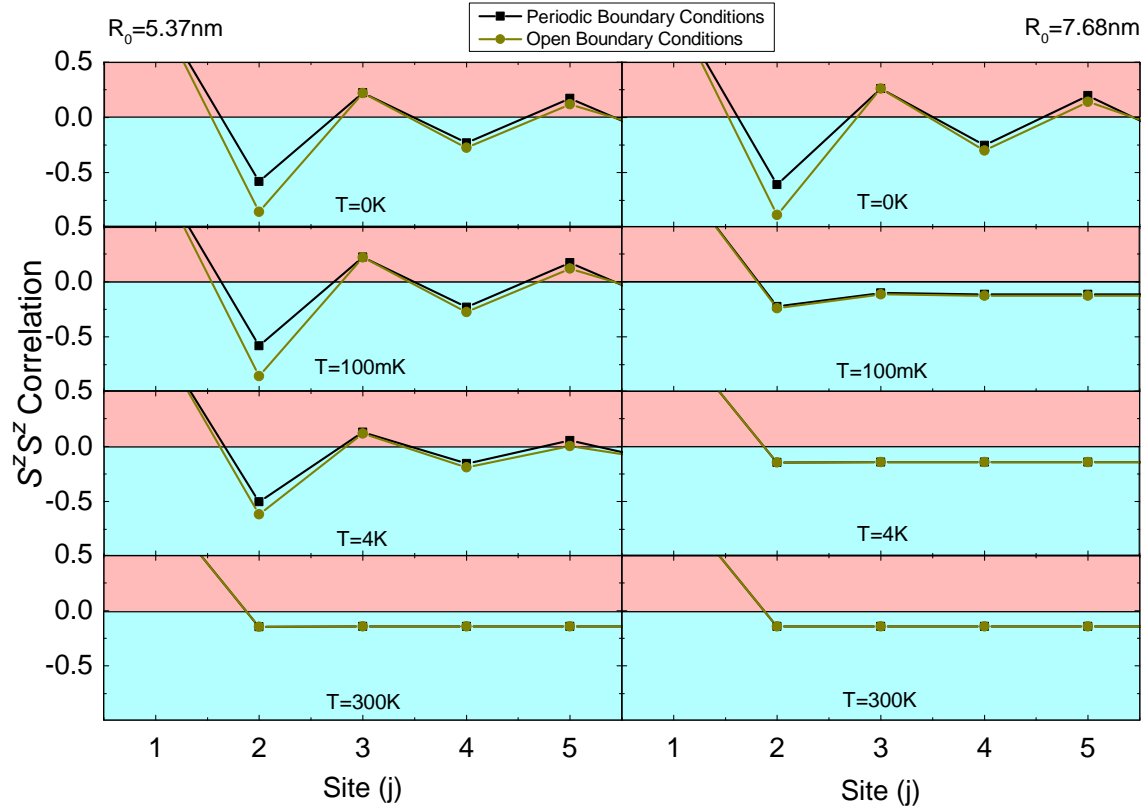


FIG. 4. Calculated $S^z S^z$ correlations for extreme temperatures, R_0 and site. The low-temperature limit corresponds to $T = 0\text{K}$, while for the high temperature limit we take arbitrarily $T = 300\text{K}$, which is not physical meaningful (see text). In all cases we compare periodic and open boundary conditions. Note that differences in the boundary conditions do not change significantly the calculated correlations and such changes do not affect our conclusions.