Self-energy correction in basis of atomic Wannier orbitals

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We present a simple scheme to map self-energy (SE) correction (SEC) of Kohn-Sham (KS) single particle states onto tight-binding (TB) parameters in the basis of Wannierized atomic orbitals. The scheme results into a SE corrected TB framework, within which, the mapping of SEC of TB parameters is found to be transferable from smaller to larger systems of similar morphology, leading to a computationally inexpensive approach for estimation of SEC in large systems with reasonable accuracy. The scheme has been demonstrated in insulating, semiconducting and magnetic nanoribbons of graphene and hexagonal boron nitride, where SEC tends strengthen the individual \(\pi\) bonds, leading to transfer of charge from edge to bulk. Additionally in magnetic bipartite systems SEC tends to enhance inter-sublattice spin separation.

Predictive designing of new materials at nanoscale, typically consisting of few tens of atoms, calls for increase in accuracy of estimation of electronic structure preferentially without a commensurate increase in computational cost. Particularly with increasing spatio-temporal resolution of syntheses, spectroscopic, and transport measurements of nanostructures, it has become imperative to match measured values to computed results in order to precisely determine structure of samples up to atomic details. Accordingly, computational methodologies have been evolved over the years for estimation of electronic structure of systems typically with a few hundreds of electrons, large enough to be within the experimentally accessible length-scales, primarily at the level of Kohn-Sham (KS) density-functional theory (DFT). As a possible approach to compute self-energy corrected energetics of electrons in such large systems, in this work we propose a tight-binding (TB) framework which incorporates effects of many-electron interactions beyond KS-DFT without involving any tunable model parameter.

Mean-field approximation of the Kohn-Sham (KS) density-functional theory (DFT), has established itself as a powerful tool for calculation of electronic structures of materials from first principles, to study ground state properties with reasonable accuracy, primarily in systems with weak localization of electrons in the valence subshells. Wannier functions, constructed from KS single particle states, have been used as TB basis to derive model Hamiltonians to focus only on the relevant group of orbitals. However, owing to the inherent lack of derivative discontinuity of the mean-field approximated exchange-correlation as local or semi-local and static functionals of density used in implementations of DFT, it undermines band-gap, overestimates binding energies while inadequately represent exchange and correlation interactions among electrons in general. Consequently, TB parameters computed from DFT often need further tuning parameters to match experimental data, such as band-gap, particularly in systems with increased correlation mainly due to localized electrons. Multitude of efforts to address these inadequacies have been pursued over the last two decades or so, within and beyond the framework of DFT. Improvement of the exchange-correlation functionals either by correcting for derivative discontinuity explicitly, or more popularly through incorporation of the inherently non-local nature of many-electron interactions by deriving non-local functionals and partial inclusion of Hartree-Fock exact exchange in hybrid functionals, have been reasonably successful in addressing particularly the issue of underestimation of band-gap by DFT, with appropriate choice of relevant parameters.

A more general parameter free approach beyond the framework of DFT, is the many-body perturbation theory (MBPT), wherein, many-electron effects are treated as perturbation, resulting into description of interacting electrons as quasi-particles (QP) whose energies include corrections to the KS single particle levels due to effective holes associated with electrons in lieu of their interaction with other electrons. These corrections, thereby known as self-energy (SE) corrections (SEC), computed up to the first order, have been shown to be sufficient in accounting for the experimentally accessible SE corrected band-gap estimated as the difference between the ionization potential (IP) and electron affinity (EA). However, since both the approaches - hybrid functionals and MBPT, are computationally expensive, MBPT being more so, it poses a severe computational challenge to compute SE corrected band-gap till date even for nanostructures with dimensions in single digits of nanometers.

In this work our approach has been to first incorporate the SEC of KS single particle levels as corrections to TB parameters in a suitable basis and subsequently see if such corrections derived from a smaller reference systems can be reasonably applied to TB parameters derived for larger systems for realistic representation of SEC in such systems without needing to explicitly compute SEC for KS states which can be computationally prohibitively expensive with growing system size. Estimate QP band-gap within a TB framework has been attempted in last few years, largely based on tuning TB parameters to match the relevant QP structure. In the following we first introduce the atomic Wannier orbitals which constitutes...
the TB basis in which SEC is mapped, followed by brief description of the GW approximation of MBPT used in this work for calculation of SEC. We demonstrate our approach in graphene nano-ribbons (GNR), where GW based SEC has been reported in detail, and also in hexagonal boron-nitride ribbons (hBNNR) as example of wide band-gap insulator.

The TB basis used in this work are orthonormal Wannier\textsuperscript{22-24} orbitals constructed as linear combination of KS energy eigen states with a specific choice of gauge that maximally retains their character as individual atomic orbitals. Since in this work we consider only 2p\textsubscript{z} orbitals we limit our discussion here on generation of one AWO per atom. We begin with a template consisting of one of the 2p orbitals each of B, C, N, and 1s of H, calculated using norm-conserving pseudo-potentials. The 2p orbital is chosen to be arbitrarily one of the 2p\textsubscript{z} orbitals since they are well known to adequately describe the edge of the valence and conduc-

Green’s functions. Within MBPT interacting electrons are represented by quasiparticles (QP) whose wavefunctions and energies satisfy the following Dyson equation involving the SE operator: 

\[ (T + V_{\text{ext}} + V_{\text{H}})\psi_{nk}'(\vec{r}) + \int d\vec{r}'\Sigma(\vec{r},\vec{r}',E_{nk})\psi_{nk}'(\vec{r}') = E_{nk}'\psi_{nk}'(\vec{r}) \]

where \( T \) is kinetic energy operator, \( V_{\text{ext}} \) is the external ionic potential, and \( V_{\text{H}} \) is the average Coulomb (Hartree) potential. We take further recourse to the GW approximation of MBPT wherein \( \Sigma \) is considered up to the first order term in its expansion, as: 

\[ \Sigma(\vec{r},\vec{r}',E) = \frac{1}{\pi} \int dE' e^{-i\delta E'} G(\vec{r},\vec{r}',E - E') W(\vec{r},\vec{r}',E'), \]

where \( \delta = 0^+ \) and the one particle non-local Green's function \( G \) is constructed in terms of the KS states \( \{ \psi_{\vec{k},n}^{KS} \} \)

The screened Coulomb interaction \( W \) is computed as: 

\[ W(\vec{r},\vec{r}',E) = \int d\vec{r}'' e^{-i\delta E''} v(\vec{r},\vec{r}'') v(\vec{r}',\vec{r}''), \]

being the bare Coulomb potential and \( e^{-1} \) being the non-local dynamic dielectric screening function. \( e^{-1} \) is computed within the random phase approximation. With the underlying assumption that correction to the KS single particle states are negligible, the quasiparticle energies are approximated as: 

\[ E_{nk}' = E_{nk}^{KS} + \langle \psi_{nk}^{KS} | \Sigma - V_{\text{xc}} | \psi_{nk}^{KS} \rangle \]

where \( V_{\text{xc}}^{KS} \) is the mean-field exchange-correlation potential derived from the exchange-correlation functionals used in DFT. Estimation of quasiparticle energies within GW approximation is computationally expensive primarily due to the slow convergence of \( e^{-1} \) and \( G \), and therefore of \( \Sigma \), with respect to unoccupied single particle KS states. Substituting \( E_{nk}^{KS} \) in Eqn(1) by quasiparticle energies \( E_{nk}' \) we calculate the SE corrected TB parameters \( \{ t_{\vec{k},\vec{k},i,j}^{QP} \} \) relevant to the quasiparticle structure. SEC of the TB parameters is thus estimated as: 

\[ \Delta t_{\vec{k},\vec{k},i,j} = t_{\vec{k},\vec{k},i,j}^{QP} - t_{\vec{k},\vec{k},i,j}^{KS} \]

where the non-self-consistent \( (G_0 W_0) \) level for estimation of quasi-particle energies using the BerkeleyGW (BGW) implementation\textsuperscript{26}. Parameters for calculation of SEC have been chosen as per Refs.\textsuperscript{27,28}. Band-gaps have been further converged with respects finer \( \vec{k} \) grid through interpolation based on the AWOs.

We consider H-passivated AGNRs and ZGNRs of varying width wherein AGNRs are specified by a number of the dimer lines and ZGNRs by the number of zigzag chains. AGNRs are categorized in three different families as per the number(n) of dimer lines: n=3p+0, n=3p+1 and n=3p+2. p being an integer. In this work we consider only the 2p\textsubscript{z} orbitals since they are well known to adequately describe the edge of the valence and conduc-
tion bands in GNRs. To maximize the 2p$_z$ character of the corresponding AWOs, sufficient participation of the anti-bonding orbitals is required in order to match the weightage of bonding orbitals, which in GNRs are represented increasingly by bonds closer to the conduction and valence band edges respectively. Fig. 1(b-f) accordingly shows convergence of $t_{ij}$ for all inequivalent atoms with respect to the total number of KS bands considered for construction of the AWOs. The fluctuation of hopping parameters from nearest to next-nearest and beyond, represent the favourable(unfavourable) nature of hopping between dissimilar(similar) sub-lattices, as generic in bipartite systems. As per Fig. 1(d), we consider in average about extra 40 unoccupied states from the valence band for construction of AWOs.

Fig. 1(g-l) shows SEC of TB parameters $\{\Delta t_{ij}\}$ for all the inequivalent atoms to their neighbours, for a representative set of AGNRs from all the three families, arranged in increasing order of width. Fig. 1(g,j,k,l) suggests that correction to nearest neighbour(n-n) hopping reduced marginally after $p=1$ and convergence beyond $p=2$. However, Fig. 1(h,g,i or h,i,j) indicates that corrections for 3p$_{+1}$ and 3p$_{+0}$ are lower than that of 3p$_{+2}$ for same $p$, consistent with the fact that AGNRs with $n=3p+2$ are inherently metallic in nature with a small gap arising exclusively due to variation in TB parameters from edge to bulk due to relaxation of bond lengths. Notably, the n-n hopping term, which is between dissimilar sub-lattices, has the most significant -ve correction implying consolidation of the n-n $\pi$-bond leading to enhanced localization of the $\pi$-bonding orbitals between atoms due to SEC. Positive correction of further hopping term between dissimilar sub-lattices also imply the same. Such localization all across the system, as implied by similar correction to hopping between nearest sites for all inequivalent atoms, would in effect result into withdrawal of charge from edge towards bulk, as evident Fig.1(f), due to consolidation of $\pi$ bonds in the bulk. The resultant overall increase in uniformity of charge distribution effectively reduces mutual Coulomb repulsion between electrons of opposite spins, leading to lowering of the on-site term due to SEC. Consistent lowering of correction to the on-site term with increasing width indicates reduced levels of SEC in general with increasing $p$. Correction to the hopping between sites within the same sub-lattice, like the hopping between next nearest sites, is negligible since it is weak in the DFT level itself.

TB Band-gap with TB parameters in AWO basis derived from KS eigen states of a given system, would match the KS band-gap of the same system by construction. Similarly, with SEC of TB parameters, referred here onwards as $\Delta t$, the correction to TB band-gap (SEC(TB)), would match the SEC of KS band-gap (SEC(KS)) of a given system, if $\Delta t$ is obtained from SEC of KS single particle levels of the same system, as evident in Fig. 2(c-e) for $p=1$ and $p=2$. Motivated by the overall similarity in SEC of TB parameters within a same family of AGNRs shown in Fig. 1(g,j,k,l), we next test if SEC(KS) of a wider AGNR with $p > 1$ can be matched by SEC(TB) estimated with TB parameters calculated from KS states of the same system ($p > 1$), but using $\Delta t$ obtained for $p=1$ ($\Delta t(p = 1)$) of the same family. The motivation to ask this question stems from the promise it holds in estimating SEC for large systems for which a direct estimation of SEC of KS band-gap can be prohibitively expensive computationally. As evident in Fig. 2(c-e), within each family, using $\Delta t(p = 1)$ and $\Delta t(p = 2)$, it is possible to account for more than 80% of SEC(KS) in wider AGNRs ($p = 3, 4$), with no appreciable increase in computational cost beyond computation of TB parameters for wider ribbons. Owing to the convergence of $\Delta t$ beyond $p=2$ [Fig. 1(g,j,k,l)], the match between SEC(TB) and SEC(KS) is more accurate with $\Delta t(p = 2)$ than with $\Delta t(p = 1)$. The scheme for assignment of $\Delta t$ from narrower to wider AGNRs is shown in Fig. 2(a-b) where the atoms of matching colors are as-

FIG. 1: For the three inequivalent atoms marked in (a): (b-f): convergence of TB parameters ($t_{ij}$) in terms of the number of KS bands considered for construction AWO(2p$_z$); (g-l): self energy correction to TB parameters ($\Delta t_{ij}$) in AGNRs of different families of increasing width.

FIG. 2: With transfer of ($\Delta t$) exemplified in (a) and (b): (b-d): comparison of band-gaps rendered by DFT,DFT+$G_0W_0$, and TB+$\Delta t$(of $p=1 & 2$) for three families of AGNRs with increasing width; (f) charge density from TB and TB+$\Delta t$. 

| $p$ | $t_{ij}$ (eV) | $\Delta t_{ij}$ (eV) |
|-----|----------------|---------------------|
| 1   | -0.9           | -0.3                |
| 2   | -0.6           | -0.3                |
| 3   | -0.3           | -0.3                |
| 4   | 0              | -0.3                |

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signed same corrections.

Next we demonstrate the scheme in hBNRs, chosen as an example of wide band gap insulator where the SEC(KS) is substantial. The difference of electronegativities of B and N are reflected in the difference in on-site terms in Fig. 3(b,c). ∆t plotted in Fig. 3(d,e) show mild +ve and strong -ve SEC for on-site terms for B and N respectively, implying enhanced polarity of the B-N π-bond and consolidation of the lone pair of N. Noticeably, unlike in GNRS, ∆t in all B and N atoms are very similar among their own kind irrespective of their proximity to edges, except the ones exactly at the edges. This is expected to enhance the degree of transferability of ∆t lacross hBN ribbons systems. Fig. 3(f) indeed suggests SEC(TB) to cover more than 90% of SEC(KS) in wider ZBNRs with ∆t calculated in the narrowest of the hBNRs considered.

We next demonstrate the scheme in ZGNRs as an example of narrow band-gap magnetic materials where Coulomb correlation plays a central role in determining the electronic structure. The difference in on-site energies [Fig. 4(b-i)] of the two spins at the zigzag edges, owes to spin separation between the two sub-lattices, which leads to localization of 2p_z electrons of opposite spins at the two edges characteristic of ZGNRs. Notably, for the C atoms at the edges, the SEC of the on-site terms Fig. 4(j-m) shows higher -ve correction for the local majority spin, compared to those of the C atoms at the interior. This implies enhanced presence of 2p_z electron of one of the spins at an edge and removal of electron of the other spin from that edge, as a result of SEC. This enhancement in spin separation across the width of ZGNRs is evident in Fig. 4(c), while Fig. 4(b) implies withdrawal of charge from edge to bulk, as seen in AGNRs as well, due to SEC. Notably, while variation in n-n hopping itself [Fig. 4(b-i)] is small among all inequivalent C atoms in each ZGNR and similar for all ZGNRs, the magnitude of ∆t for n-n hopping reduces from Z12 to Z16 and converged thereafter [Fig. 4(j-i)] for both spins. Accordingly, Fig. 4(b) suggests a better accounting of SEC(KS) of wider ZGNRs(Z20,Z24) using ∆t of Z16 than that using ∆t of Z12.

Pertinently, transfer of charge from edge to bulk as seen in Fig. 4(b), accompanied by enhancement of localization of opposite spins near the edges seen in Fig. 4(c), is also observed within the Hubbard model with increasing strength of the on-site Coulomb repulsion U, although it is clear from the contribution of off-diagonal terms of ∆t in reproducing SEC(KS), that DFT+U alone will not be sufficient to account for SEC. However, unlike AGNRs, ZGNRs being magnetic systems, it is reasonable to anticipate that SEC of KS single particle states will also have impact on the on-site Coulomb repulsion term U in addition to TB parameters. Therefore while substituting ∆t of wider ZGNRs by that of Z12 or Z16, we need to account for a possible underestimation of U. We therefore take recourse to the mean field approximation of the Hubbard model and self-consistently introduce ∆U along with ∆t, as $H = \sum_{i,j,\sigma} (t_{ij} + \Delta t_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + ...
\[ \sum_{i,\sigma} \Delta U_{i,\sigma} n_{i,\sigma'} \{ t_{ij} \} \] are computed from KS eigen states of the wider ZGNRs\((Z20,Z24)\), and \(\{ \Delta t_{ij} \} \) from Z16. \( \Delta U \) is tuned to match SEC(TB) to SEC(KS) in Z20 and Z24. As evident in Fig�(a), indeed with application of a small \( U \) in addition to the \( \Delta \) \( \text{U} \), eigen states of the wider ZGNRs\((Z20,Z24)\), and \{ \( i_{ij} \} \) are computed from KS \{ \( t \} \) which is with \( U=0 \).

In conclusion, we have presented a computationally inexpensive scheme for estimation of self-energy correction(SEC) of band-gap within a tight-binding(TB) framework in the basis of atomic Wannier orbitals (AWO) constructed from KS energy eigen states. Within the scheme, SEC of TB parameters are first computed for a smaller reference systems from SEC of KS single particle levels estimated using the GW approximation of MBPT, and then applied to TB parameters derived for a larger system of similar morphology, in order to estimate SEC of KS band-gap of the larger system, without needing to explicitly compute it. The efficacy of the approach, demonstrated in semiconducting and insulating as well as magnetic and non-magnetic nano-ribbons of graphene and hexagonal boron-nitride, is found to account for about 90% or more of the SE corrected band-gap for 50% to 100% increase in system size as assessed in this work, with nominal increase in computational cost. In general, the SEC corrected TB framework opens the scope for in-depth analysis of SEC without having to explicitly generate SE corrected KS states. The results presented here pave the way for building up a repository of self-energy corrected TB parameters of different atoms at different chemical environment for their seamless use in estimation of SEC within a multi-orbital TB framework.

\[ \sum_{i,\sigma} \Delta U_{i,\sigma} n_{i,\sigma'} \{ t_{ij} \} \] where \{ \( t_{ij} \} \) are computed from KS eigen states of the wider ZGNRs\((Z20,Z24)\), and \(\{ \Delta t_{ij} \} \) from Z16. \( \Delta U \) is tuned to match SEC(TB) to SEC(KS) in Z20 and Z24. As evident in Fig�(a), indeed with application of a small \( U \) in addition to the \( \Delta \) \( \text{U} \), eigen states of the wider ZGNRs\((Z20,Z24)\), and \{ \( i_{ij} \} \) are computed from KS \{ \( t \} \) which is with \( U=0 \).

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