

Supplementary Material

The calculation of the bond orbital matrix elements within the BPT approach $V_B = \langle \mathcal{X} | \hat{V}_B | \mathcal{X} \rangle$ over hybrids (see manuscript eq. (1 b)) requires computing a sum of pseudo two centre integrals:

$$\left\langle \mathcal{X} \left| \frac{Q_x}{|\bar{R}_x - \bar{r}|} \right| \mathcal{X} \right\rangle = \sum_k h_k^2 \int \phi_k(\bar{r}) \frac{Q_x}{|\bar{R}_x - \bar{r}|} \phi_k(\bar{r}) d\bar{r}^3$$

The charges are centred at the sites X, and the hybrids are located at the positions of A or B. The hybrid coefficients h are calculated from the geometry of the bond system. Slater type atomic orbitals are used to derive simple analytic formulas for the integrals – see Table 1.

Atomic Orbitals		$\left\langle \phi_{nlm} \left \frac{1}{ \bar{R} - \bar{r} } \right \phi_{n'l'm'} \right\rangle$
$\langle ns $	$ ns\rangle$	$\frac{1}{R}$
$\langle p_z $	$ np_z\rangle$	$\frac{1}{R} + \frac{1}{R^3} \frac{(2n+1)(2n+2)}{5(2\zeta)^2} (3\cos^2(\theta) - 1)$
$\langle ns $	$ np_z\rangle$	$-\frac{2}{\sqrt{3}R^3} \frac{(2n+1)\sqrt{(2\zeta_1)^{2n+1}(2\zeta_2)^{2n+1}}}{(\zeta_1 + \zeta_2)^{2n+2}} \cos(\theta)$
$\langle np_x $	$ np_x\rangle$	$\frac{1}{R} + \frac{1}{R^3} \frac{(2n+1)(2n+2)}{2 \cdot 5 \cdot (2\zeta)^2} [3(1 - \cos^2(\theta))\cos(2\varphi) - (3\cos^2(\theta) - 1)]$
$\langle np_y $	$ np_y\rangle$	$\frac{1}{R} - \frac{1}{R^3} \frac{(2n+1)(2n+2)}{2 \cdot 5 \cdot (2\zeta)^2} [3(1 - \cos^2(\theta))\cos(2\varphi) + (3\cos^2(\theta) - 1)]$

Table 1: Integrals over Slater type atomic orbitals for sp^2 and sp^3 bonded atoms. These integrals are needed for the calculation of bond polarization energies.

The knowledge of atomic charges is of substantial interest; and there several methods to calculate this atomic property, i.e. ESP (charges derived from electrostatic potentials) (1), MPA (Mulliken population analysis) (2), DI (density integration) (3), NPA (natural

population analysis) (4), ENC (electronegativity charges) (5) or PACHA (partial atomic charges and hardness analysis) (6). Several models: NPA, MPA, ESP, PACHA and ENC were applied to a pseudopeptide zinc complex (7) consisting of 64 atoms (H, C, N, O, Zn). The structure was optimized with GAUSSIAN 98 (8) applying density functional theory with a 6-31G(d,p) basis set. The charge calculations were carried out with best performance parameters (NPA with a 6-31G basis set, MPA and ESP with a 3-21G basis set). PACHA charges were calculated by Marc Henry (private communication) and ENC with the COSMOS program (9). The results of these models were correlated and compared with each another. The following correlation matrix was obtained (left to right and top to bottom: NPA, MPA, ESP, PACHA and ENC)

$$\begin{pmatrix} 1 & 0.963 & 0.871 & 0.941 & 0.853 \\ 0.963 & 1 & 0.845 & 0.845 & 0.755 \\ 0.871 & 0.845 & 1 & 0.815 & 0.796 \\ 0.941 & 0.845 & 0.815 & 1 & 0.934 \\ 0.853 & 0.755 & 0.796 & 0.934 & 1 \end{pmatrix}$$

The comparison of NPA charges with PACHA charges yields a correlation coefficient of 0.941 for instance. The best correlation is observed between NPA and MPA: the correlation coefficient is 0.963. The data was further analyzed by a multivariate normal distribution with the density function

$$P(\bar{Q}) = \frac{1}{2\pi\sqrt{\det[C^{-1}]}} \exp\left[-\frac{1}{2}(\bar{Q} - \bar{q})^T C^{-1}(\bar{Q} - \bar{q})\right],$$

covariance matrix elements

$$C_{ij} = \overline{Q_i Q_j} - \overline{Q_i} \overline{Q_j},$$

and hence resulted:

$$C = e^2 \begin{pmatrix} 0.228 & 0.183 & 0.182 & 0.078 & 0.102 \\ 0.183 & 0.159 & 0.148 & 0.058 & 0.074 \\ 0.182 & 0.148 & 0.192 & 0.062 & 0.086 \\ 0.078 & 0.058 & 0.062 & 0.03 & 0.04 \\ 0.102 & 0.074 & 0.086 & 0.04 & 0.061 \end{pmatrix}$$

The vector $\bar{Q} = (q_1, q_2, q_3, q_4, q_5) = (q_{NPA}, q_{MPA}, q_{ESP}, q_{PACHA}, q_{ENC})$ is the vector of charge models, and \bar{q} is the corresponding vector of means. The covariance matrix C is symmetric, and a transformation in the principal value system is performed. The coordinate system is changed by a rigid rotation to remove any correlations between the variables in q_i :

$$(\bar{Q} - \bar{q})^T T^T \begin{pmatrix} 0.609 & 0 & 0 & 0 & 0 \\ 0 & 0.034 & 0 & 0 & 0 \\ 0 & 0 & 0.023 & 0 & 0 \\ 0 & 0 & 0 & 0.004 & 0 \\ 0 & 0 & 0 & 0 & 0.001 \end{pmatrix} T (\bar{Q} - \bar{q}),$$

$$(\bar{Q}' - \bar{q}') = T (\bar{Q} - \bar{q})$$

with the transformation matrix

$$T = \begin{pmatrix} -0.270 & -0.220 & -0.235 & -0.092 & -0.123 \\ 0.172 & 0.183 & -0.368 & 0.034 & -0.026 \\ 0.044 & -0.214 & -0.094 & 0.165 & 0.341 \\ 0.245 & -0.245 & 0.023 & 0.139 & -0.245 \\ 0.197 & -0.119 & -0.009 & -0.375 & 0.079 \end{pmatrix}.$$

The eigenvector corresponding to the largest eigenvalue having the smallest variance, has the form

$$q_1' \sim (q_{NPA} + 0.87 q_{ESP} + 0.81 q_{MPA} + 0.46 q_{ENC} + 0.34 q_{PACHA}).$$

Due to the large eigenvalue of $0.609/e^2$, which corresponds to the smallest variance of $1.64e^2$ or a standard deviation of $1.28e$, this coordinate dominates all other coordinates q'_i . NPA has a

major contribution to the eigenvector and the probability distribution which can be approximated by

$$P(\bar{Q}) \approx P(\bar{Q}_1') = \frac{1}{2\pi\sqrt{1.64}} \exp\left[-\frac{1}{2} \frac{(\bar{Q}_1' - \bar{q}_1')^2}{1.64e^2}\right].$$

NPA is the charge calculation model of choice judged by the statistical investigation above. In this work, the BPT was parameterized using the methods NPA, ESP and MPA to test for best performance. The models PACHA and ENC were not employed for three reasons: i) They showed a low contribution to the eigenvector q'_l , ii) they cannot be calculated by *ab initio* techniques and iii) they are less coordinate dependent than the BPT formalism.

For the BPT parameterization, a set of 175 model structures including 12 zinc compounds were optimized with DFT/B3LYP applying a 6-31G(d,p) basis set. The calibration was done in two steps. First, a subset of 163 molecules consisting of H, C, N, O, F, Si, P, S and Cl was employed for calibration testing 11 different basis sets for best performance (best correlation with BPT). In a second step, the best basis sets, that are also applicable to Zn-calculations, were used for the calibration with a set of 175 structures.

Mulliken Population Analysis (MPA)

The simplest and most common approximate *ab initio* treatment is SCF-MO-LCAO-CGTO (Self Consistent Field approach of Molecular Orbitals that are approximated as Linear Combinations of Atomic Orbitals using Contracted Gauss Type Orbitals). The SCF closed shell molecular wave function of N electrons is approximated from the CI or CC model as

$$|\Psi\rangle = \sum_l C_l |\Psi_l\rangle \approx |\Psi_1\rangle ,$$

using an anti-symmetric sum of products of N molecular spin orbitals $|\Phi_i(j)\rangle$

$$|\Psi\rangle \approx \frac{1}{\sqrt{N!}} \sum_P (-1)^P \hat{P} [|\Phi_1(1)\rangle |\Phi_1(2)\rangle \cdots |\Phi_1(N)\rangle] ,$$

with $|\Phi_i(2k-1)\rangle = |\alpha_i(k)\rangle|\chi_i(k)\rangle$, $|\Phi_i(2k)\rangle = |\beta_i(k)\rangle|\chi_i(k)\rangle$ and $k = 1 \dots N/2$. \hat{P} is the permutation operator. The molecular orbitals $|\chi_i(k)\rangle$ are approximated as LCAOs (Linear Combination of Atomic Orbitals) of STOs. In order to understand a population analysis, the local density operator at atom position A is defined as

$$\hat{\rho}_A = |\bar{r}_A\rangle\langle\bar{r}_A|,$$

with $\sum_A \hat{\rho}_A = 1$. The local density is given by

$$\begin{aligned} \rho_A &= \langle\Psi|\bar{r}_A\rangle\langle\bar{r}_A|\Psi\rangle \\ &= \left(\sum_i^{N/2} (\langle\alpha_i(k)| + \langle\beta_i(k)|) |\chi_i(k)\rangle |\bar{r}_A\rangle \right) \left(\sum_j^{N/2} \langle\bar{r}_A|\chi_j(l)\rangle (|\alpha_j(l)\rangle + |\beta_j(l)\rangle) \right) \\ &= 2 \sum_i^{N/2} \langle\chi_i(k)|\bar{r}_A\rangle\langle\bar{r}_A|\chi_j(l)\rangle \\ &= 2 \sum_i^{N/2} \sum_{\mu,\nu} c_{i\mu}^* c_{i\nu} \phi_\mu^*(\bar{r}_{A(k)}) \phi_\nu^*(\bar{r}_{A(l)}). \end{aligned}$$

Defining the bond-order matrix \hat{D} with its matrix elements as $D_{\mu\nu} = 2 \sum_i^{N/2} c_{i\mu}^* c_{i\nu}$, it follows

$$\rho_A = \sum_{\mu,\nu} D_{\mu\nu} \phi_\mu^*(\bar{r}_{A(k)}) \phi_\nu^*(\bar{r}_{A(l)})$$

Thus, the population at atom A can be calculated by

$$\begin{aligned} N_A &= \int \rho_A dV \\ &= \sum_{\mu,\nu} D_{\mu,\nu} S_{\mu,\nu} \\ &= \sum_{\mu}^A \left(D_{\mu\mu} + \sum_{\nu,\mu \neq \nu}^A D_{\mu,\nu} S_{\mu,\nu} + \sum_{B,A \neq B} \sum_{\nu,\mu \neq \nu} D_{\mu,\nu} S_{\mu,\nu} \right), \end{aligned}$$

with $S_{\mu\nu} = \int \phi_\mu^*(\bar{r}_{A(k)}) \phi_\nu(\bar{r}_{A(l)}) dV$, and the atomic charge can be defined as

$$Q_A = e(Z_A - N_A) .$$

There are two problems connected with the MPA (2). First, the overlap contribution, called interference density, $\sum_B \sum_{\nu, \mu \neq \nu}^B D_{\mu, \nu} S_{\mu, \nu}$ of atom A to all other atoms B is equally distributed to A as well as B, which is an inadequate assumption for strongly polarized hetero-atomic bonds. Second, problems arise in case of delocalized contributions which describe the electron density of A, $\sum_{\mu}^A D_{\mu\mu}$. This effect is strongly basis set dependent.

MPA			
	R	SD [e]	$SD/\Delta Q$ [%]
STO-2G	0.9912	0.0247	13.15
STO-3G	0.9911	0.0247	13.22
STO-6G	0.9944	0.0244	10.50
3-21G	0.9941	0.0448	10.77
6-21G	0.9941	0.0439	10.80
6-31G(d,p)	0.9917	0.0391	12.73
6-31+G(,p)	0.9583	0.1036	27.38
6-31++G(d,p)	0.9325	0.1325	33.69
6-311G(d,p)	0.9850	0.0476	16.98
6-311G+(d,p)	0.8466	0.1322	45.06
6-311G++(d,p)	0.8182	0.1463	47.05

Table 2: Basis set dependence of the MPA charge parameterization of BPT with basis sets (first column), correlation coefficients R (second column) compared to *ab initio* charges, standard deviation SD (third column), ratios of the standard deviation and the absolute charge distribution deviation ΔQ (last column).

The extreme dependence of the Mulliken charges on the basis set is illustrated in the following example: The second carbon atom of CH_2CFCl has a positive charge (+0.05 e) calculated with a 3–21G basis set, it is negatively charged (-0.11e) when calculated with a 6–311++G(d,p) basis.

A sum of one-electron operators for MPAs can be defined

$$\hat{Q}_A^{MPA} = e \left(Z_A - \sum_i^A |\phi_i, \sigma(i)\rangle \langle \phi_i, \sigma(i)| \right) .$$

This is important, because BPT assumes one-electron operators.

A first parameterization applying STO-3G Mulliken charges were done by Sternberg et al. (10, 11). The best correlation (correlation coefficient $R=0.9944$) is achieved with a STO-6G basis set, see Table 2. This basis set not applicable to Zn, since it is incomplete in GAUSSIAN98. Therefore, the basis set with the second best correlation (3-21G) was applied for necessary charge calculations to parameterize the BPT method on 175 molecules including 12 zinc structures. The correlation coefficient is 0.9933, the standard deviation is 0.05 e. The BPT parameters q_i and A_i , are given in Table 3.

MPA-Parameter		MPA-Parameter	
q(C=O)	0.17211	q(H-N)	0.26131
A(C=O)	1.59284	A(H-N)	0.3906
A(C=C)	0.74459	q(C-F)	0.30133
q(C=N)	0.20782	A(C-F)	-0.06306
A(C=N)	2.14726	q(Cl-C)	0.23255
q(P=O)	0.19201	A(Cl-C)	0.0112
A(P=O)	0.15857	q(Si-H)	0.12036
q(S=O)	-0.29007	A(Si-H)	1.44897
A(S=O)	-0.19149	q(Si-C)	0.28795
q(S=C)	0.07191	A(Si-C)	0.89486
A(S=C)	0.99008	q(Si-O)	0.46332
q(P-O)	0.21615	A(Si-O)	-1.0826
A(P-O)	0.83216	q(Si-Cl)	0.25731
q(S-O)	0.75986	A(Si-Cl)	3.34254
A(S-O)	2.94333	q(S-H)	-0.10449
q(C-N)	0.14506	A(S-H)	-1.16316
A(C-N)	-0.77123	A(S-S)	2.03518
A(C-C)	0.36218	q(S-C)	0.26439
q(C-O)	0.25771	A(S-C)	-0.43828
A(C-O)	-1.38054	q(Zn-N)	0.24496
q(H-O)	0.33601	A(Zn-N)	4.33392
A(H-O)	0.26976	q(Zn-O)	0.39707
q(H-C)	0.19878	A(Zn-O)	-0.14277
A(H-C)	0.30287		

Table 3: BPT parameters of MPA/3-21G (q_i in e and A_i in e/H).

Electrostatic Charges (ESP)

A totally different approach is used to compute partial charges via the molecular electrostatic potential which is evaluated at points in space around the molecule, and the data are fitted to a classical atomic point charge model (1). The fitting parameters are the charges. The number of layers and the density of points per unit area are input parameters. In this work 10 layers and 10 points per unit area were used since these parameters gave good results within a reasonable computational time.

ESP	R	SD [e]	$SD/\Delta Q$ [%]
STO-2G	0.9597	0.0824	26.97
STO-3G	0.9595	0.0825	27.04
STO-6G	0.9659	0.0832	25.03
3-21G	0.9768	0.0818	20.93
6-21G	0.9758	0.0820	21.34
6-31G(d,p)	0.9668	0.0813	24.71
6-31+G(d,p)	0.9414	0.1155	31.75
6-31++G(d,p)	0.9426	0.1137	31.46
6-311G(d,p)	0.9470	0.1081	30.43
6-311G+(d,p)	0.9427	0.1172	31.44
6-311G++(d,p)	0.9427	0.1171	31.47

Table 4: Basis set dependence of the ESP charge parameterization of BPT with basis sets (first column), correlation coefficients compared to *ab initio* charges are listed R (second column), standard deviations SD (third column), ratios of the standard deviation and the absolute charge distribution deviation ΔQ (last column).

There is no sum of one-electron operators for ESPs defined which makes its theoretical application within the BPT approach uncertain, since BPT parameters cannot be correctly interpreted. Nevertheless, the parameterization was carried out in respect to different basis sets. The results are given in Table 4. The correlations are not as good as the calculations done using MPA. The best parameterization is obtained with a 3-21G basis set, $R=0.9768$. The complete parameterization of the 175 structures was performed employing a 3-21G basis set and ESP. The correlation coefficient is 0.9721 with a standard deviation of 0.08 e. The obtained BPT parameters are given in Table 5.

ESP-Parameter		ESP-Parameter	
q(C=O)	0.19053	q(H-N)	0.19726
A(C=O)	2.40837	A(H-N)	3.13988
A(C=C)	3.13028	q(C-F)	0.18888
q(C=N)	-0.12967	A(C-F)	1.1354
A(C=N)	4.49582	q(Cl-C)	-0.00286
q(P=O)	0.55216	A(Cl-C)	1.70729
A(P=O)	0.11158	q(Si-H)	0.11869
q(S=O)	-1.20227	A(Si-H)	5.0306
A(S=O)	2.20363	q(Si-C)	0.09691
q(S=C)	-0.03686	A(Si-C)	2.70133
A(S=C)	1.79232	q(Si-O)	0.37292
q(P-O)	-0.15059	A(Si-O)	1.0639
A(P-O)	2.75509	q(Si-Cl)	0.21257
q(S-O)	1.11203	A(Si-Cl)	6.16056
A(S-O)	-0.1139	q(S-H)	-0.24591
q(C-N)	0.06987	A(S-H)	-2.06931
A(C-N)	2.83202	A(S-S)	7.40194
A(C-C)	2.52632	q(S-C)	-0.05875
q(C-O)	0.20341	A(S-C)	0.90494
A(C-O)	-0.64017	q(Zn-N)	0.11386
q(H-O)	0.40384	A(Zn-N)	4.48369
A(H-O)	0.32417	q(Zn-O)	0.69723
q(H-C)	0.10118	A(Zn-O)	2.23474
A(H-C)	1.89935		

Table 5: BPT parameters of ESP/3-21G (q_i in e and A_i in e/H).

Natural Population Analysis (NPA)

The natural population analysis method was formulated by Reed et al. (4). It is based on the fact that the non-orthogonal atomic orbitals $\{\phi_k\}$ can be transformed to ortho-normal NAOs (Natural Atomic Orbitals) $\{\psi_\mu\}$

$$\psi_\mu = \sum_k T_{k\mu} \phi_k$$

Due to this property of the NAOs, the overlap matrix elements vanishes for different orbitals

$$S_{\mu\nu} = \int \phi_{\mu}^*(\vec{r}_{A(k)}) \phi_{\nu}(\vec{r}_{A(l)}) dV = \delta_{\mu\nu}$$

and the population at atom A can be calculated:

$$N_A = \sum_{\mu}^A D_{\mu\mu}.$$

NPA			
	R	SD [e]	SD/ΔQ [%]
STO-2G	0.9955	0.0449	9.41
STO-3G	0.9878	0.0308	15.35
STO-6G	0.9928	0.0290	11.91
3-21G	0.9960	0.0437	8.89
6-21G	0.9960	0.0435	8.91
6-31G(d,p)	0.9967	0.0437	8.12
6-31+G(d,p)	0.9893	0.0774	14.40
6-31++G(d p)	0.9897	0.0748	14.14
6-311G(d,p)	0.9896	0.0710	14.24
6-311G+(d,p)	0.9795	0.0959	19.69
6-311G++(d,p)	0.9796	0.0958	19.68

Table 6: Basis set dependence of the NPA charge parameterization of BPT with basis sets (first column), correlation coefficients compared to *ab initio* charges are listed *R* (second column), standard deviations *SD* (third column), ratios of the standard deviation and the absolute charge distribution deviation ΔQ (last column).

The overlap matrix elements and interference terms vanish. These are big advantages in comparison to MPA. Problems arise in case of less localized basis sets, since delocalized contributions of the wave functions describe the electron density of a neighbouring atom causing errors in the description. Therefore, compact basis sets should be employed. A sum of one-electron operators of NPAs can be defined from the population N_A using the natural spin atomic orbitals by

$$\hat{Q}_A^{NPA} = e \left(Z_A - \sum_i^A |\psi_i, \sigma(i)\rangle \langle \psi_i, \sigma(i)| \right).$$

The parameterization results (of 163 structures) can be seen in Table 6. The 6–31G(d,p) basis set gave the best correlation ($R=0.9967$). The same basis set was applied for the parameterization including the 12 Zn-structures which yielded a correlation coefficient of 0.9961 with a standard deviation of 0.05 e. The BPT parameters q_i and A_i for effective charge calculation are given in Table 7.

NPA-Parameter		NPA-Parameter	
q(C=O)	0.24732	q(H-N)	0.38172
A(C=O)	1.48918	A(H-N)	0.27397
A(C=C)	0.59962	q(C-F)	0.39704
q(C=N)	0.13766	A(C-F)	-0.58294
A(C=N)	1.13287	q(Cl-C)	0.04777
q(P=O)	0.47328	A(Cl-C)	-0.00124
A(P=O)	0.14528	q(Si-H)	0.14891
q(S=O)	-0.98019	A(Si-H)	2.17524
A(S=O)	0.13009	q(Si-C)	0.38416
q(S=C)	-0.09903	A(Si-C)	1.08137
A(S=C)	1.29061	q(Si-O)	0.63482
q(P-O)	0.29554	A(Si-O)	-0.12469
A(P-O)	0.37048	q(Si-Cl)	0.3487
q(S-O)	1.49458	A(Si-Cl)	1.741996
A(S-O)	3.29897	q(S-H)	-0.16454
q(C-N)	0.12007	A(S-H)	-0.26373
A(C-N)	-0.97646	A(S-S)	3.21091
A(C-C)	0.53831	q(S-C)	0.15962
q(C-O)	0.29676	A(S-C)	-0.10032
A(C-O)	-1.39582	q(Zn-N)	1.04517
q(H-O)	0.47641	A(Zn-N)	-7.8104
A(H-O)	0.15249	q(Zn-O)	0.17456
q(H-C)	0.22781	A(Zn-O)	12.85987
A(H-C)	0.44427		

Table 7: BPT parameters of NPA/6-31G(d,p) (q_i in e and A_i in e/H).

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