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Theoretical Study of Charge Mobility Properties of Complexes Si(DPP)(CH$_3$)$_2$ and Si(Bzimpy)(CH$_3$)$_2$

The direction of organic electronics research is attracting more and more interest from the scientific community. One of the indicators of such interest is the appearance of commercially available products with screens based on organic compounds. Therefore, conducting experimental and theoretical research in this area is an urgent task. Pentacoordination neutral complexes of silicon are poorly studied from the point of view of application in organic electronics, as well as six-coordination analogues. We present data on the calculation of reorganization energies, intermolecular transfer integrals, transfer rates and charge mobility for the optimized structures of pentacoordinated silicon complexes Si(DPP)(CH$_3$)$_2$ and Si(bzimpy)(CH$_3$)$_2$. We have applied Marcus-Hush model for calculation of charge mobilities. The Si(DPP)(CH$_3$)$_2$ structure contains one diphenylpyridine (DPP = 2,6-diphenylperidine) ligand. The Si(bzimpy)(CH$_3$)$_2$ structure contains one benzimidazole (bzimpy = 2,6-bis(benzimidazole-2'-il)pyridine) ligand. Computational data were obtained using the B3LYP hybrid functional and the basis set 6-31G*. All calculations were performed using Gaussian09 program package. The charge mobility data obtained for Si(DPP)(CH$_3$)$_2$ and Si(bzimpy)(CH$_3$)$_2$ pentacoordinated silicon complexes were compared with their six-coordinate counterparts Si(DPP)$_2$ and Si(bzimpy)$_2$ for which experimental data on charge mobilities become available last years. Comparison with six-coordination analogues of complexes showed that penta-coordination complexes Si(DPP)(CH$_3$)$_2$ and Si(bzimpy)(CH$_3$)$_2$ have much higher mobility of electrons, while Si(bzimpy)(CH$_3$)$_2$ also has higher hole mobility. We suppose this could be related to different symmetry of the pentacoordinated and hexacoordinted complexes. It is shown that the mobility of holes is much higher in the complex Si(bzimpy)(CH$_3$)$_2$ than in Si(DPP)(CH$_3$)$_2$.

Keywords: density functional method DFT, silicon pentacoordinated complexes, pyridine-containing ligands, charge mobility, reorganization energy, internal reorganization energy, intermolecular transfer integral, charge transfer rate, charge carrier diffusion coefficient.

Introduction

In recent years, there has been considerable interest in the study of light emitting diodes based on organic materials, which are usually called organic light emitting diodes (OLEDs) [1, 2]. But at the same time, a huge wave of commercial success creates a great need to improve the efficiency, stability and sustainability of new materials [3]. The need is exacerbated by recent advances in organic electronics [4–6]. Organic semiconductors also find application in various organic photovoltaic (OPV) [7–10] and OLED [11–14] devices, in particular as a hole conduction layer (HTL) [15, 16] or as an electronic conduction layer (ETL) [17]. It is worth to mention that hexacoordinated silicon complexes have shown remarkable stability [18, 19].

At the moment pentacoordinated silicon complexes are new type of molecules that attract scientists due to their properties. They can also be used in organic electronics, allowing improvements to existing devices that are of interest for further research. The desire to improve the physical properties of materials led to the study of charge transport characteristics. Determination of structural-functional relationships between the mobility of electrons and holes is of high importance for the development of efficient devices. In this work, the objects of study are pentacoordination silicon complexes: Si(DPP)(CH$_3$)$_2$ containing one diphenylpyridine ligand and Si(bzimpy)(CH$_3$)$_2$ with a benzimidazole ligand. The purpose of this work is a theoretical study of the properties of charge transport in these compounds using the density functional theory.

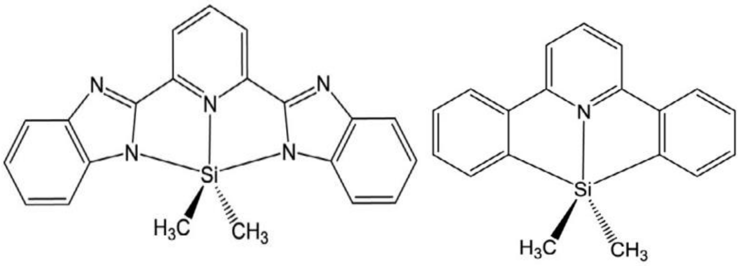


Figure 1. Left — 2D structure of $Si(bzimpy)(CH_3)_2$ complex, right — 2D structure of $Si(DPP)(CH_3)_2$ complex

Computational Details

For quantum-chemical studies, models of the $Si(DPP)(CH_3)_2$ and $Si(bzimpy)(CH_3)_2$ structures were built, for which the DFT (density functional theory method) method implemented in the GaussianW09 Rev.E01 software package was used [20]. This software package includes a wide range of different functionals. In our calculations we have used B3LYP hybrid functional [21–23]. Subsequently, the structures were optimized using the basis set: 6-31G* [24–27]. An analysis of the nature of the molecular orbitals, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), has been studied. Calculations of vibrational frequencies showed the absence of negative values, which indicates that all the obtained structures correspond to the absolute minimum of energy.

Results and Discussion

We have obtained optimized structures of $Si(DPP)(CH_3)_2$ and $Si(bzimpy)(CH_3)_2$. Tables 1 and 2 demonstrate basic geometrical parameters of optimized molecules $Si(DPP)(CH_3)_2$ and $Si(bzimpy)(CH_3)_2$.

Table 1

Data on geometrical parameters of optimized $Si(bzimpy)(CH_3)_2$

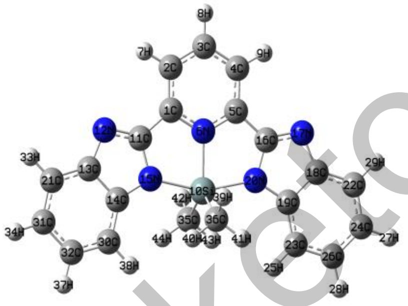
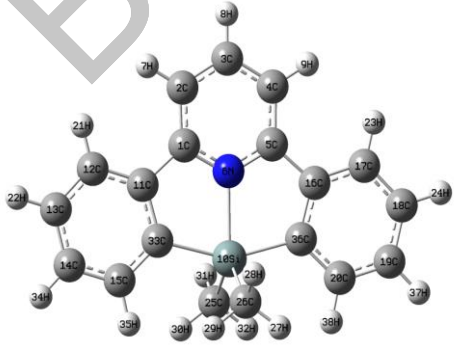
$Si(bzimpy)(CH_3)_2$	Bond length (Å)		Angles (º)	
	^{10}Si-^{6}N	1.94032	^{10}Si-^{6}N-^{1}C	119.239
	^{10}Si-^{35}C	1.88533	^{1}C-^{11}C-^{15}N	113.439
	^{10}Si-^{15}N	1.92868	^{11}C-^{15}N-^{10}Si	117.116
	^{6}N-^{1}C	1.35863	^{6}N-^{1}C-^{2}C	120.439
	^{15}N-^{14}C	1.37820	^{1}C-^{2}C-^{3}C	118.372
	^{1}C-^{2}C	1.39367	^{11}C-^{15}N-^{14}C	103.805
	^{2}C-^{7}H	1.08330	^{15}N-^{11}C-^{12}N	116.957
	^{13}C-^{14}C	1.43169	^{14}C-^{13}C-^{21}C	120.271
	^{31}C-^{32}C	1.41447	^{6}N-^{10}Si-^{35}C	119.432

Table 2

Data on geometrical parameters of optimized $Si(DPP)(CH_3)_2$

$Si(DPP)(CH_3)_2$	Bond length (Å)		Angles (º)	
	^{10}Si-^{6}N	2.12188	^{10}Si-^{6}N-^{1}C	118.139
	^{10}Si-^{36}C	1.98610	^{1}C-^{11}C-^{33}C	114.041
	^{10}Si-^{26}C	1.91774	^{6}N-^{10}Si-^{33}C	76.733
	^{6}N-^{1}C	1.34211	^{11}C-^{33}C-^{10}Si	119.004
	^{15}C-^{14}C	1.37820	^{1}C-^{2}C-^{3}C	118.336
	^{1}C-^{2}C	1.39976	^{6}N-^{1}C-^{2}C	119.371
	^{2}C-^{7}H	1.08395	^{1}C-^{6}N-^{5}C	123.721
	^{13}C-^{14}C	1.39847	^{13}C-^{14}C-^{15}C	120.251
	^{11}C-^{33}C	1.40953	^{33}C-^{10}Si-^{26}C	97.194

Next, we have calculated energies of reorganization of holes λ_{hole} and electrons $\lambda_{electron}$ for the molecules using formula (1) [28–30]. Reorganization energies are summation of relaxation energies during the transition from neutral molecule to cation/anion and back on potential energy surfaces.

$$\lambda_{hole} = [E{+}(A) - E{+}(A{+})] + [E(A{+}) - E(A)],$$
$$\lambda_{electron} = [E{-}(A) - E{-}(A{-})] + [(A{-}) - (A)], \quad (1)$$

where $E(A)$ — energy of neutral molecule after optimization; $E(A+)$ — energy of cation of a molecule after optimization; $E+(A+)$ — energy of positively charged molecule with the geometry of a neutral molecule; $E+(A)$ — energy of a neutral molecule with geometry of cation; $E(A–)$ — energy of an anion after optimization; $E–(A–)$ — energy of negatively charged molecule with the geometry of a neutral molecule; $E–(A)$ — energy of a neutral molecule with the geometry of an anion.

Tables 3 and 4 demonstrate data for calculation of reorganization energies of charges for the molecules Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$.

Table 3

Data for calculation of reorganization energies of holes in Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$

Molecule	$E(A)$ (eV)	$E(A+)$ (eV)	$E+(A+)$ (eV)	$E+(A)$ (eV)	λ_{hole} (eV)
Si(bzimpy)$(CH_3)_2$	–37368.9106	–37361.9183	–37361.8213	–37368.8130	0.0006
Si(DPP)$(CH_3)_2$	–29336.2819	–29329.6028	–29338.9966	–29333.9283	11.7474

Table 4

Data for calculation of reorganization energies of electrons in Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$

Molecule	$E(A)$ (eV)	$E(A–)$ (eV)	$E–(A–)$ (eV)	$E–(A)$ (eV)	$\lambda_{electron}$ (eV)
Si(bzimpy)$(CH_3)_2$	–37368.9106	–37370.2840	–37370.0787	–37368.7221	–0.0168
Si(DPP)$(CH_3)_2$	–29336.2819	–29336.7976	–29336.5080	–29336.0409	–0.0486

On the next step we have estimated energies of HOMO and LUMO. Figures 2 and 3 represent visualized HOMO and LUMO for molecules Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$. As one can see from Figures 2 and 3 HOMOs and LUMOs are formed by π orbitals of the ligands.

Figure 4 demonstrate boundary MOs energy levels diagram of molecules Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$. According to Figure 4 both molecules have about the same energy of HOMO but different energies of LUMO. Therefore, band gap in Si(bzimpy)$(CH_3)_2$ is about 2.7 eV while for Si(DPP)$(CH_3)_2$ it is about 4 eV.

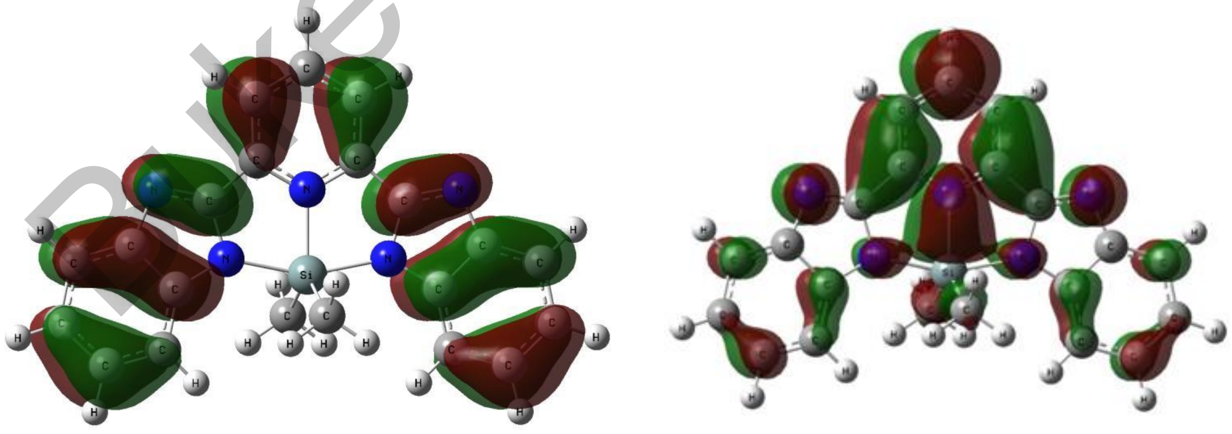


Figure 2. Visualized HOMO (left) and LUMO (right) of the complex Si(bzimpy)$(CH_3)_2$

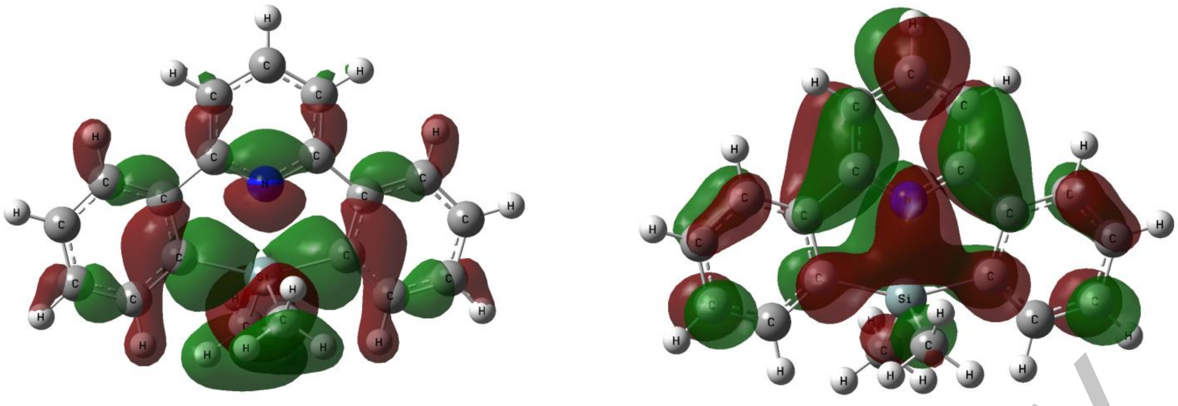


Figure 3. Visualized HOMO (left) and LUMO (right) of the complex Si(DPP)$(CH_3)_2$

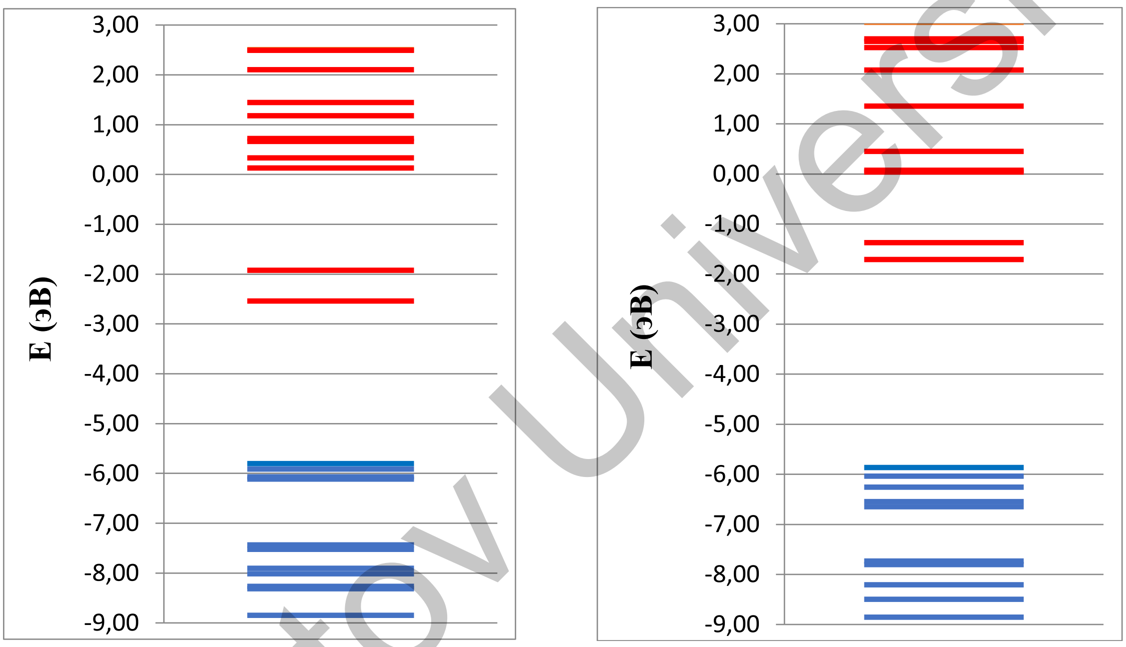


Figure 4. Energy levels diagram of boundary MOs for the molecules Si(bzimpy)$(CH_3)_2$ (left) and Si(DPP)$(CH_3)_2$ (right). Blue color indicates occupied MOs and red indicates unoccupied MOs

Using Koopmans theorem approximation and energy splitting in dimer method we have used formula (2) for calculation of the integral of intermolecular charge transfer $V_{h/e}$ for holes and electrons [31–33]:

$$V_{h/e} = \frac{\varepsilon_{H[L+1]} - \varepsilon_{H-1[L]}}{2}, \qquad (2)$$

where $\varepsilon_{H[L+1]}$ — energy of HOMO (LUMO+1); $\varepsilon_{H-1[L]}$ — energy of HOMO-1 (LUMO) in dimer. In order to perform these calculations we have optimized structures of dimers for Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$ molecules. Figures 5 and 6 demonstrate optimized structures of the dimers. For these dimers structures we have calculated energies of frontier MO energies. Figure 7 demonstrates diagram of MOs for the dimers.

Table 5 demonstrates data for energies of HOMO-1, HOMO, LUMO и LUMO+1 for calculation of $V_{h/e}$.

Table 5

Data for calculation of $V_{h/e}$ for the compounds Si(bzimpy)$(CH_3)_2$ and Si(DPP)$(CH_3)_2$

Molecule	E_{HOMO} (eV)	E_{HOMO-1} (eV)	V_{hole} (eV)	E_{LUMO} (eV)	E_{LUMO+1} (eV)	$V_{electron}$ (eV)
Si(bzimpy)$(CH_3)_2$	–5.78272	–5.84283	0.030055	–2.49696	–2.47139	0.012785
Si(DPP)$(CH_3)_2$	–5.92525	–6.05472	0.064735	–1.75821	–1.56509	0.09656

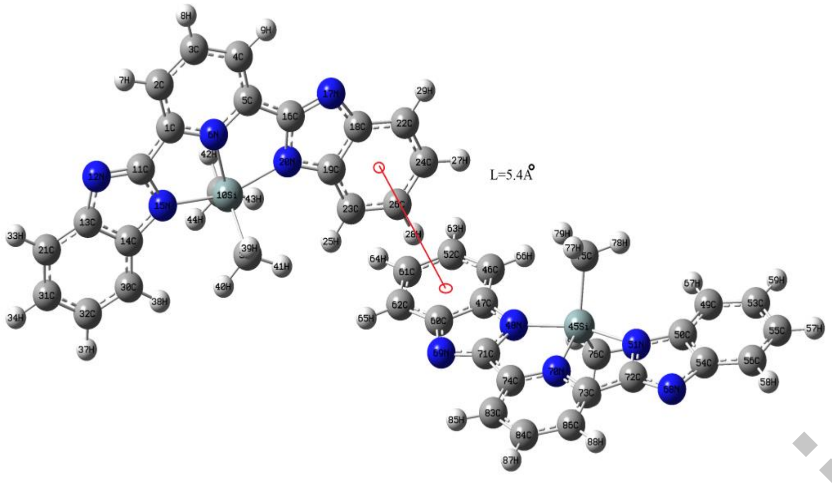


Figure 5. Structure of dimer for molecule Si(bzimpy)$(CH_3)_2$

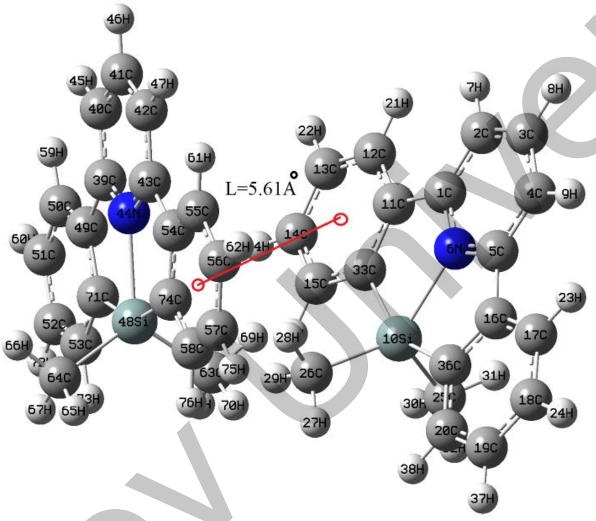


Figure 6. Structure of dimer for molecule Si(DPP)$(CH_3)_2$

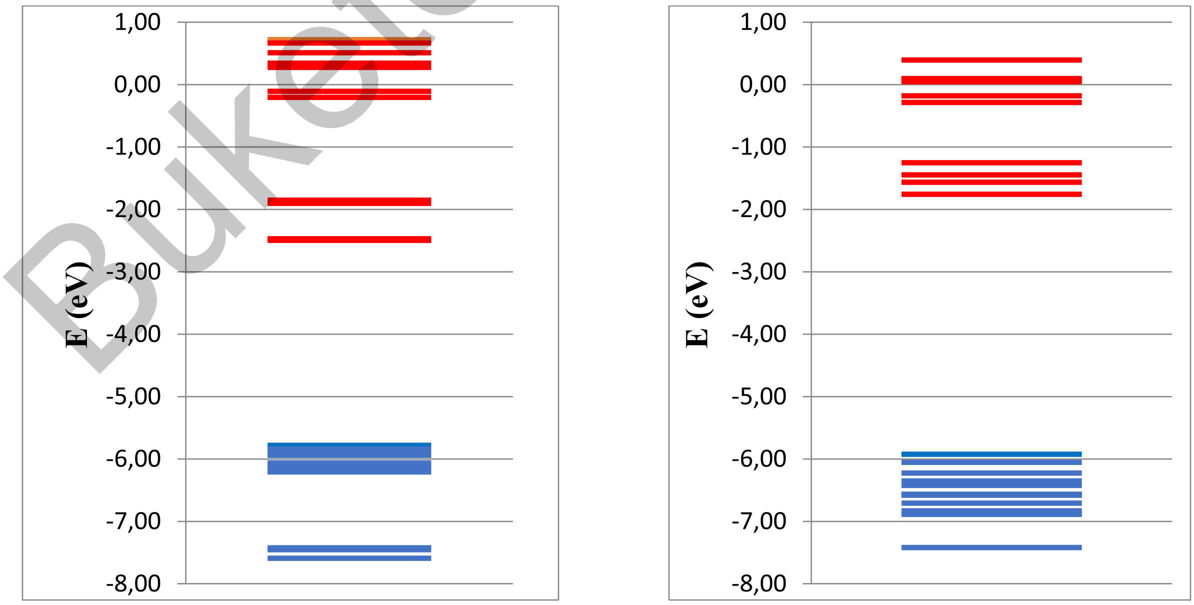


Figure 7. Energy levels diagram of boundary MOs for the dimers of Si(bzimpy)$(CH_3)_2$ (left) and Si(DPP)$(CH_3)_2$ (right). Blue color indicates occupied MOs and red indicates unoccupied MOs

Next, we have calculated transfer rate of holes and electrons $\mathrm{Ket}_{h/e}$ which is described by the formula (3) in accordance with Marcus-Hush theory [34, 35]:

$$\mathrm{Ket}_{h/e} = \sqrt{\frac{\pi}{\lambda_{h/e} k_B T}} \cdot \frac{V_{h/e}^{\ 2}}{\hbar} \cdot \exp\left(-\frac{\lambda_{h/e}}{4K_B T}\right), \qquad (3)$$

where k_B — Boltzmann constant; T — temperature, $\hbar$ — Plank constant, $\lambda_{h/e}$ — reorganization energy of hole and electron.

Using data obtained above and known constants we have calculated transfer rates for the molecules. Table 6 demonstrates data for $\mathrm{Ket}_{h/e}$. As one can see from Table 6 transfer rate for holes in $Si(DPP)(CH_3)_2$ is very small. This is mostly due to large value of λ_{hole} in $Si(DPP)(CH_3)_2$.

Table 6

Calculated transfer rates for $Si(bzimpy)(CH_3)_2$ and $Si(DPP)(CH_3)_2$

Molecule	Ket hole (s^{-1})	Ket electron (s^{-1})
$Si(bzimpy)(CH_3)_2$	$6.21\times10^{+14}$	1.81×10^{13}
$Si(DPP)(CH_3)_2$	6.79×10^{-38}	4.43×10^{14}

In order to estimate diffusion coefficient of charge carriers it is necessary to know the distance between molecules in a dimer. Therefore, we have estimated distance between molecules in the dimers for molecules $Si(bzimpy)(CH_3)_2$ and $Si(DPP)(CH_3)_2$. Figures 5 and 6 demonstrate distances between the molecules.

The diffusion coefficient could be estimated based on the Einstein-Smoluchowski formula [36]:

$$D = \frac{L^2 \mathrm{Ket}}{2}, \qquad (4)$$

where Ket — charge transfer rate, L — distance between molecules in a dimer. Using calculated values of Ket and L we have obtained D values for holes and electrons, which are shown in Table 7.

Table 7

Charge carriers diffusion coefficients for molecules $Si(bzimpy)(CH_3)_2$ and $Si(DPP)(CH_3)_2$

Molecule	L (Å)	D_{hole} ($cm^2\ s^{-1}$)	$D_{electron}$ ($cm^2\ s^{-1}$)
$Si(bzimpy)(CH_3)_2$	5.40	9.05×10^{-1}	2.64×10^{-2}
$Si(DPP)(CH_3)_2$	5.61	1.07×10^{-52}	6.97×10^{-1}

In a weak field approximation charge mobility could be estimated by the Einstein formula [37]:

$$\mu = \frac{eD}{kT}, \qquad (5)$$

where e — electron charge, D — diffusion coefficient of charge carriers. Using obtained data from above we have calculated charge mobilities for the molecules. Table 8 demonstrates calculated charge mobilities.

Table 8

Charge carriers mobilities for molecules $Si(bzimpy)(CH_3)_2$ and $Si(DPP)(CH_3)_2$

Molecule	μ_{hole} ($cm^2\ V^{-1}\ s^{-1}$)	$\mu_{electron}$ ($cm^2\ V^{-1}\ s^{-1}$)
$Si(bzimpy)(CH_3)_2$	3.58×10^{1}	1.04×10^{0}
$Si(DPP)(CH_3)_2$	4.23×10^{-51}	2.76×10^{1}

According to the obtained results, presence of bzimpy ligand provides much higher value of hole mobility in comparison with DPP ligand, and DPP ligand provides higher electron mobility than bzimpy in the considered molecules. To estimate relatively values of $\mu_{hole/electron}$ we may mention experimental data for sixcoordinated analogues $Si(DPP)_2$ [38] $\mu_{hole} = 1.1\times10^{-5}$ ($cm^2\ V^{-1}\ s^{-1}$), $\mu_{electron} = 18\times10^{-5}$ ($cm^2\ V^{-1}\ s^{-1}$) and $Si(bzimpy)_2$ $\mu_{hole} = 5.31\times10^{-6}$ ($cm^2\ V^{-1}\ s^{-1}$), $\mu_{electron} = 9.68\times10^{-5}$ ($cm^2\ V^{-1}\ s^{-1}$) [39]. Comparison of charge mobilities for pentacoordinated and sixcoordinated silicon analogues demonstrates that pentacoordinated $Si(bzimpy)(CH_3)_2$ has much higher values, while $Si(DPP)(CH_3)_2$ has high electron mobility and very low hole mobility. This could be due to lower symmetry of pentacoordinated silicon compounds in comparison with highly symmetrical sixcoordinated ones.

Conclusions

In this paper we have considered properties of charge transport in neutral pentacoordinated silicon complexes Si(DPP)$(CH_3)_2$ and Si(bzimpy)$(CH_3)_2$ using DFT method. For the molecule Si(bzimpy)$(CH_3)_2$ we have shown that hole mobility is higher than for electrons. Our calculations for Si(DPP)$(CH_3)_2$ have demonstrated very low mobility of holes. The comparison of the results obtained for compounds Si(DPP)$(CH_3)_2$ and Si(bzimpy)$(CH_3)_2$ has demonstrated that Si(bzimpy)$(CH_3)_2$ has higher charge mobility for holes than Si(DPP)$(CH_3)_2$ while Si(DPP)$(CH_3)_2$ has higher electron mobility. Also, we have compared the values of $\mu_{\text{hole/electron}}$ for pentacoordinated and sixcoordinated complexes with ligands bzimpy and DPP and it was revealed that pentacoordinated analogues have much lower values of charge mobilities. We believe that this fact is related to high symmetry of sixcoordinated silicon complexes.

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