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Simulation and modeling of organic thermoelectric materials for waste heat regeneration

Resonant modes due to electron-phonon coupling in dopped polythiophene

```
(*We write firstly well-known matrix elements of the model*)
```

```
α̃1 = 0.0; α̃2 = 0.0; α̃3 = 0.0; α̃4 = 0.0; α̃6 = 0.0;
α̃7 = 0.0; α̃8 = 0.0; α̃9 = 0.0; α̃11 = 0.0; s = -4.0;
(*α̃i is ionization potential of C atom
 and s standing for the same quantity for S atom,
tilda stands to indicate modification of ionization energy due to disorder,
here undopped values have been taken into account*)


A = 123.6; B = 0.3776; c0 = 7.814;
(*static lattice parameters taken from PRL 1989,vol.63,7,786-789*)
Rcc = 1.557; Rcs = 1.782;
(* p=1 takes into account interaction with phonons,i.e. for p=0,
phonon-electron coupling is absent and the calculation goes for static lattice*)
p = 1.0;
 (*p=1 takes into account interaction with phonons,i.e. for p=0,
phonon-electron coupling is absent and the calculation goes for static lattice*)
```

$$\beta 12 = A * Exp\left[-\frac{1.441}{B}\right] + p * c0 * A * Exp\left[-\frac{1.441}{B}\right] * (1.441 - Rcc + B);$$

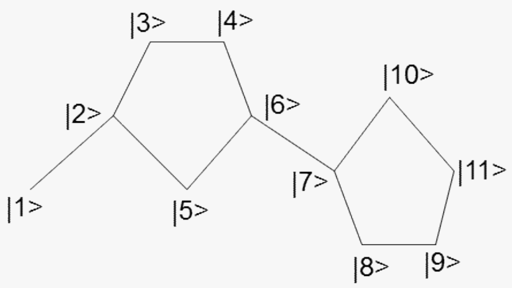
$$\beta 23 = A * Exp\left[-\frac{1.457}{B}\right] + p * c0 * A * Exp\left[-\frac{1.457}{B}\right] * (1.457 - Rcc + B);$$

$$\beta 34 = A * Exp\left[-\frac{1.350}{B}\right] + p * c0 * A * Exp\left[-\frac{1.350}{B}\right] * (1.350 - Rcc + B);$$

$$\beta 25 = A * Exp\left[-\frac{1.721}{B}\right] + p * c0 * A * Exp\left[-\frac{1.721}{B}\right] * (1.721 - Rcs + B);$$

```
 (*first part are bonds, the second expresses phonon correction. Rij
 are taken from Table I from aforementioned reference *)
Import["C:\\Users\\gor\\Desktop\\imagePT.pdf"]
```

polythiophene-MONOMER in atomic basis, any other conjugated polymer is applicable as well



We write Hamiltonian of the monomer system on the atomic basis from off-diagonal elements defined above as follows

$$M = \begin{pmatrix} \tilde{\alpha}1 & \beta 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta 12 & \tilde{\alpha}2 & \beta 23 & 0 & \beta 25 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \beta 23 & \tilde{\alpha}3 & \beta 34 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta 34 & \tilde{\alpha}4 & 0 & \beta 23 & 0 & 0 & 0 & 0 & 0 \\ 0 & \beta 25 & 0 & 0 & s & \beta 25 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta 23 & \beta 25 & \tilde{\alpha}6 & \beta 12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \beta 12 & \tilde{\alpha}7 & \beta 23 & 0 & \beta 25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta 23 & \tilde{\alpha}8 & \beta 34 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta 34 & \tilde{\alpha}9 & 0 & \beta 23 \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta 25 & 0 & 0 & s & \beta 25 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta 23 & \beta 25 & \tilde{\alpha}11 \end{pmatrix};$$

Then we introduce Hamiltonian for the sparse polymer system

```
Poly101 = MatrixForm[
  SparseArray[{Band[{1, 1}] → M, Band[{11, 12}] → β12, Band[{12, 11}] → β12,
    Band[{12, 12}] → M, Band[{22, 23}] → β12, Band[{23, 22}] → β12,
    Band[{23, 23}] → M, Band[{33, 34}] → β12, Band[{34, 33}] → β12,
    Band[{34, 34}] → M, Band[{44, 45}] → β12, Band[{45, 44}] → β12,
    Band[{45, 45}] → M, Band[{55, 56}] → β12, Band[{56, 55}] → β12,
    Band[{56, 56}] → M, Band[{66, 67}] → β12, Band[{67, 66}] → β12,
    Band[{67, 67}] → M, Band[{77, 78}] → β12, Band[{78, 77}] → β12,
    Band[{78, 78}] → M, Band[{88, 89}] → β12, Band[{89, 88}] → β12,
    Band[{89, 89}] → M, Band[{100, 101}] → β12,
    Band[{101, 100}] → β12, Band[{101, 101}] → α̃1}, {101, 101}]];
```

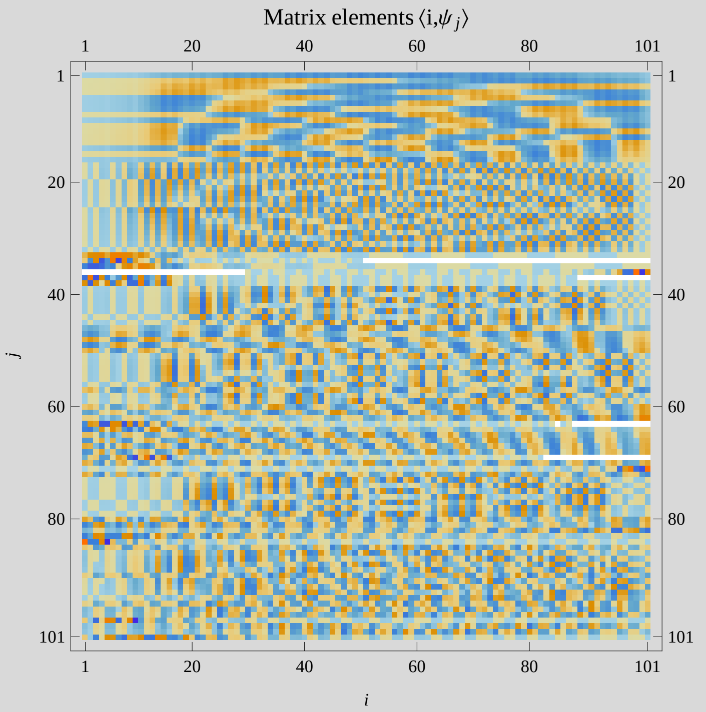
```
(*Eigen problem is solved in next step
 for static polymer intercting with phonons*)
```

```
{vals, vecs} = Eigensystem[%]
```

```
dat1 = vals;
dat2 = vecs;
```

For each eigenstate $|\psi_j\rangle = \sum_{i=1}^{101} \langle i || \psi_j \rangle \mid i\rangle$ which are novel dressed electronic states due to disorder and coupling to phonons we can plot coefficients $\langle i || \psi_j \rangle$ in atomic basis

```
pic1 = MatrixPlot[vecs, FrameLabel → {j, i}, PlotLabel → "Matrix elements 〈i,ψj〉"]
```

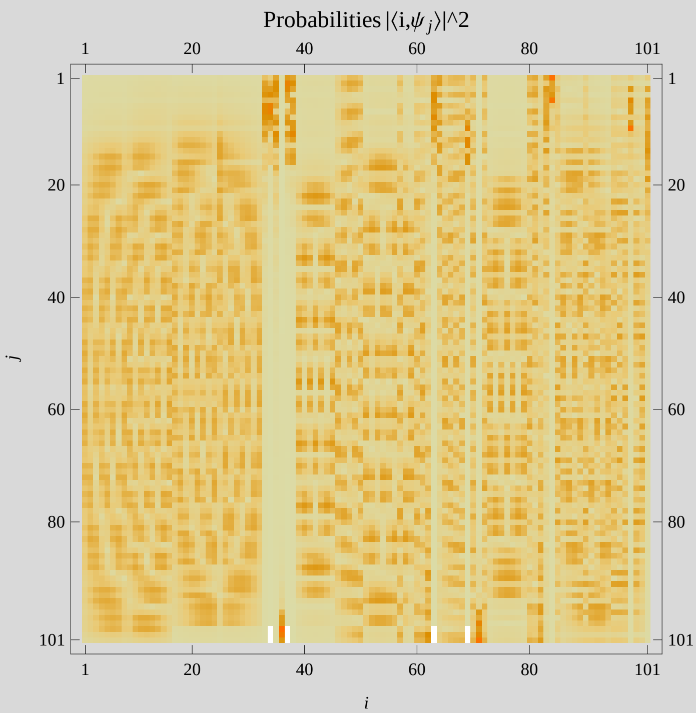



```
data3 = Table[vecs[[i]], {i, 1, 101}]
```

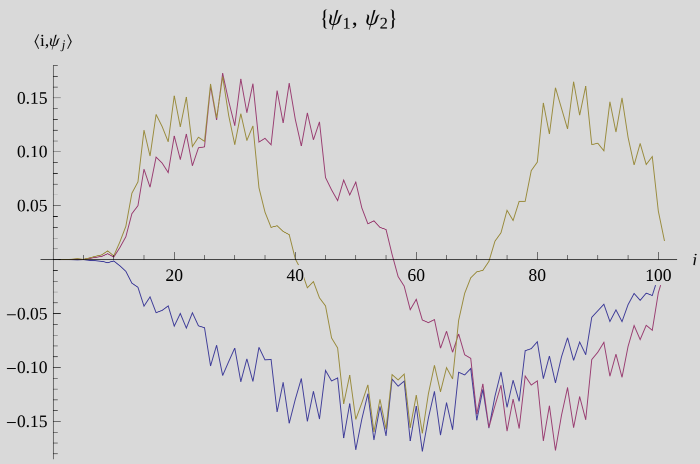
```
data4 = Table[vecs[[i, j]] * vecs[[i, j]], {j, 1, 101}, {i, 1, 101}];
```

```
MatrixForm[data4]
```

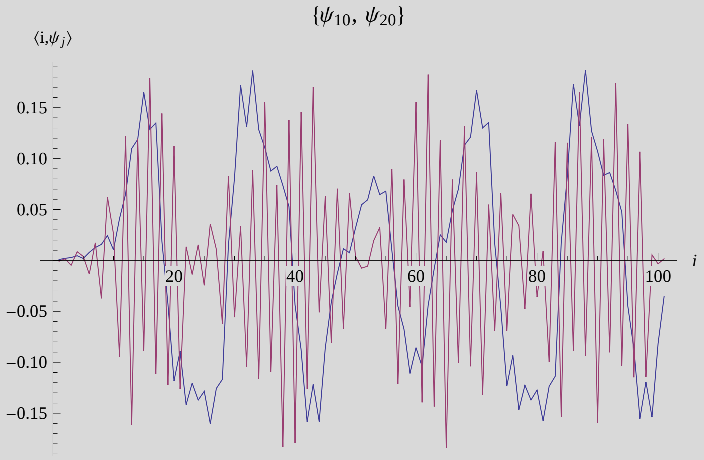
```
pic2 = MatrixPlot[%, FrameLabel → {j, i}, PlotLabel → "Probabilities |⟨i,ψj⟩|^2"]
```



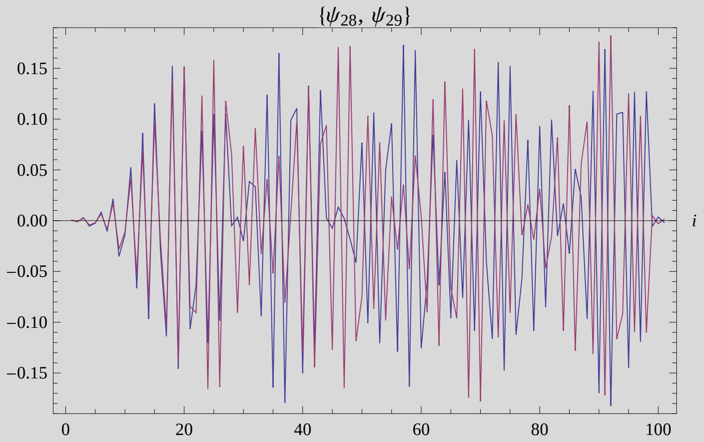

```
im1 = ListLinePlot[{vecs[[1]], vecs[[2]], vecs[[3]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ1, ψ2}]
```



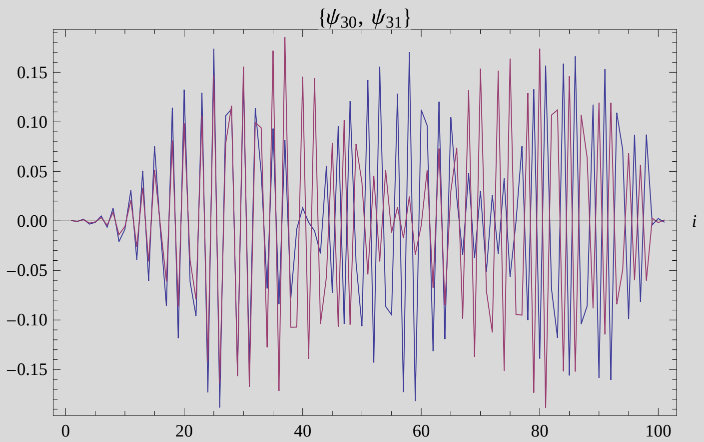
```
im2 = ListLinePlot[{vecs[[10]], vecs[[20]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ10, ψ20}]
```




```
im3 = ListLinePlot[{vecs[[28]], vecs[[29]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ28, ψ29}, Frame → True]
```




```
im4 = ListLinePlot[{vecs[[30]], vecs[[31]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ30, ψ31}, Frame → True]
```



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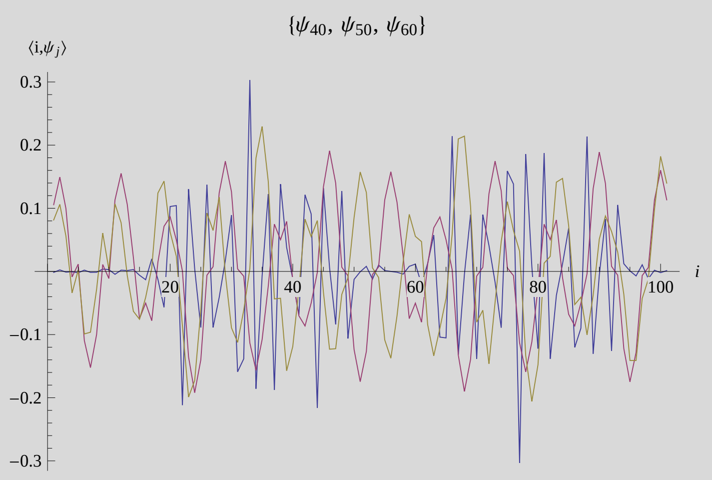
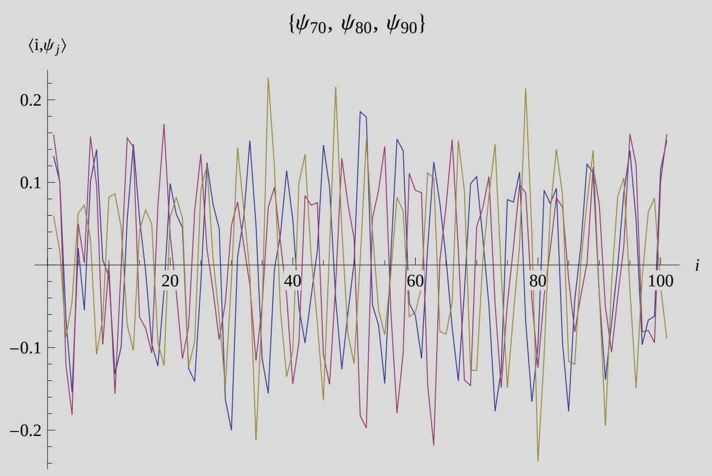
```
im5 = ListLinePlot[{vecs[[40]], vecs[[50]], vecs[[60]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ40, ψ50, ψ60}]
```




```
im6 = ListLinePlot[{vecs[[70]], vecs[[80]], vecs[[90]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ70, ψ80, ψ90}]
```




```
im7 = ListLinePlot[{vecs[[100]], vecs[[101]]},
  AxesLabel → {i, "⟨i,ψj⟩"}, PlotLabel → {ψ100, ψ101}]
```