

**Supplementary Materials of**  
**“Exciton diffusion in poly(3-hexylthiophene) by first-principles molecular dynamics”**  
**by Cheick Oumar Diarra, Mauro Boero, Emilie Steveler, Thomas Heiser and Evelyne Martin**

CPMD input file

```
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  Dynamical simulation of first principles dynamics within the ROKS framework
  Exemple of input file
&END

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  ROKS
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  WANNIER OPTIMIZATION JACOBI
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  SUBTRACT ROTVEL
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  NOSE ELECTRONS
  0.033 5000.0
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  TRAJECTORY SAMPLE XYZ
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  RESTFILES
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  REAL SPACE WFN KEEP
  CENTER MOLECULE ON
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  PBE
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&ATOMS

\*S\_MT\_PBE.psp KLEINMAN-BYLANDER

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-2.2945996545	3.5261604278	3.0997786822
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\*C\_MT\_PBE.psp KLEINMAN-BYLANDER

LMAX=P

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\*H\_MT\_PBE.psp KLEINMAN-BYLANDER

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