

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Differential charge density-CNF.

File Name: Supplementary Data 2

Description: Differential charge density-ONF.

File Name: Supplementary Data 3

Description: Molecular electrostatic potential-CNF.

File Name: Supplementary Data 4

Description: Molecular electrostatic potential-ONF.

File Name: Supplementary Data 5

Description: Binding energies of PVDF with I_3^- .

File Name: Supplementary Data 6

Description: Binding energies of PVDF with I_5^- .

File Name: Supplementary Data 7

Description: Binding energies of CNF with I_3^- .

File Name: Supplementary Data 8

Description: Binding energies of CNF with I_5^- .

File Name: Supplementary Data 9

Description: Binding energies of ONF with I_3^- .

File Name: Supplementary Data 10

Description: Binding energies of ONF with I_5^- .

File Name: Supplementary Data 11

Description: Gibbs free energy of PVDF- $3I_2$.

File Name: Supplementary Data 12

Description: Gibbs free energy of PVDF- $2I_3^-$.

File Name: Supplementary Data 13

Description: Gibbs free energy of PVDF- $6I^-$.

File Name: Supplementary Data 14

Description: Gibbs free energy of CNF- $3I_2$.

File Name: Supplementary Data 15
Description: Gibbs free energy of CNF-2I₃⁻.

File Name: Supplementary Data 16
Description: Gibbs free energy of CNF-6I⁻.

File Name: Supplementary Data 17
Description: Gibbs free energy of ONF-3I₂.

File Name: Supplementary Data 18
Description: Gibbs free energy of ONF-2I₃⁻.

File Name: Supplementary Data 19
Description: Gibbs free energy of ONF-6I⁻.

File Name: Supplementary Data 20
Description: Molecular dynamics simulation of CNF-25.

File Name: Supplementary Data 21
Description: Molecular dynamics simulation of CNF-40.

File Name: Supplementary Data 22
Description: Molecular dynamics simulation of ONF-25.

File Name: Supplementary Data 23
Description: Molecular dynamics simulation of ONF-40.