

Quantum Espresso DFT/PBE energies for the optimized structures, attached as .cif files. Structures not discussed in manuscript (less stable ones, saddle points, converged to already discussed geometry from different initial points) included in subdirectories 'OtherStructures'.

Cluster models cut from selected periodic structures and used for ORCA TDDFT/LC-BLYP/ma-def2-TZVP calculations attached as .xyz files.

S₄Na₈Sod models

```

cisC2v_S4Na8Ssod
!    total energy                =    -1778.96144662 Ry
Cs_S4Na8Ssod
!    total energy                =    -1778.91389529 Ry
transC1_S4Na8Ssod              (initial structure: transC2h)
!    total energy                =    -1778.88136482 Ry
D2d_S4Na8Ssod
!    total energy                =    -1778.87579487 Ry
D3h_S4Na8Ssod
!    total energy                =    -1778.86489615 Ry

Other structures:
cisC2v_S4Na8Ssod_2             converged to cisC2v_S4Na8Ssod
!    total energy                =    -1778.96139065 Ry
D2h_S4Na8Ssod                  converged to transition state
!    total energy                =    -1778.92198306 Ry
D2h_S4Na8Ssod_2                converged to cisC2v_S4Na8Ssod
!    total energy                =    -1778.96131482 Ry
D3h_S4Na8Ssod
!    total energy                =    -1778.86337701 Ry
transC2h_S4Na8Ssod_2           converged to cisC2v_S4Na8Ssod
!    total energy                =    -1778.96117673 Ry
C3v_S4Na8Ssod                  converged to another D3h structure
!    total energy                =    -1778.86371329 Ry

```

S₄Na₇Clsod models

cisC2v_S4Na7Clsod

! total energy = -1694.38592586 Ry

Cs_S4Na7Clsod

! total energy = -1694.33717074 Ry

transC2h_S4Na7Clsod

! total energy = -1694.31285609 Ry

D2d_S4Na7Clsod

! total energy = -1694.31454243 Ry

D3h_S4Na7Clsod

! total energy = -1694.28926004 Ry

Other structures:

D2h_S4Na7Clsod converged to cisC2v_S4Na7Clsod

! total energy = -1694.38580225 Ry

cisC2v_S4Na7Clsod_2 converged to cisC2v_S4Na7Clsod

! total energy = -1694.38440400 Ry

transC2h_S4Na7Clsod_2

! total energy = -1694.30713766 Ry

D2d_S4Na7Clsod_2

! total energy = -1694.30989018 Ry

D3h_S4Na7Clsod_2

! total energy = -1694.28817789 Ry