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.

$S_4^-Na_8Clsod$ models

```
cisC2v_S4-Na8Clsod          (initial structure transC2h)
!    total energy              =   -1790.70173671 Ry
cisC2v_S4-Na8Clsod_2
!    total energy              =   -1790.69066727 Ry
twistC2_S4-Na8Clsod         (initial structure transC2h)
!    total energy              =   -1790.66209306 Ry
C3v_S4-Na8Clsod
!    total energy              =   -1790.64319182 Ry
Cs_S4-Na8Clsod
!    total energy              =   -1790.63687210 Ry


Other Structures:
D2h_S4-Na8Clsod             converged to D2 symm. saddle point
!    total energy              =   -1790.66984459 Ry
D2h_S4-Na8Clsod_2           converged to cisC2v_S4-Na8Clsod-2
!    total energy              =   -1790.69053775 Ry
cisC2v_S4-Na8Clsod_3        converged to cisC2v_S4-Na8Clsod-2
!    total energy              =   -1790.69048509 Ry*
D2d_S4-Na8Clsod             converged to D2 symm. saddle point
!    total energy              =   -1790.66577121 Ry
D3h_S4-Na8Clsod
!    total energy              =   -1790.64319590 Ry
```

$S_4^-Na_7sod$ models

```
cisC2v_S4-Na7sod_1
!    total energy              =   -1662.25286530 Ry
cisC2v_S4-Na7sod_2         (initial structure transC2h)
!    total energy              =   -1662.23565485 Ry
C3v_S4-Na7sod
!    total energy              =   -1662.18612439 Ry

Other Structures:
cisC2v_S4-Na7sod_3    converged to transition state
                           (initial structure transC2h)
!    total energy              =   -1662.24451613 Ry
D2h_S4-Na7sod_1       converged to cisC2v_S4-Na7sod_1
!    total energy              =   -1662.25272270 Ry
D2h_S4-Na7sod_2       converged to cisC2v_S4-Na7sod_1
!    total energy              =   -1662.23565485 Ry
C3v_S4-Na7sod_2            (initial structure D3h)
!    total energy              =   -1662.18609670 Ry
```