

-- Supporting information for --

# **Cl@Si<sub>20</sub>X<sub>20</sub> cages. Evaluation of Encapsulation Nature, Structural Rigidity, and <sup>29</sup>Si-NMR Patterns from Relativistic DFT Calculations**

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Figure S1. Contour plot representation of NICS, z- and y-component of the induced magnetic field,  $B_z^{\text{ind}}$  and  $B_y^{\text{ind}}$ , for Si<sub>20</sub>H<sub>20</sub>, Si<sub>20</sub>H<sub>12</sub>Cl<sub>8</sub>, and, Si<sub>20</sub>Cl<sub>20</sub>. Page 2

Table S1. Coordinates for optimized structures in multiXYZ format. Page 3

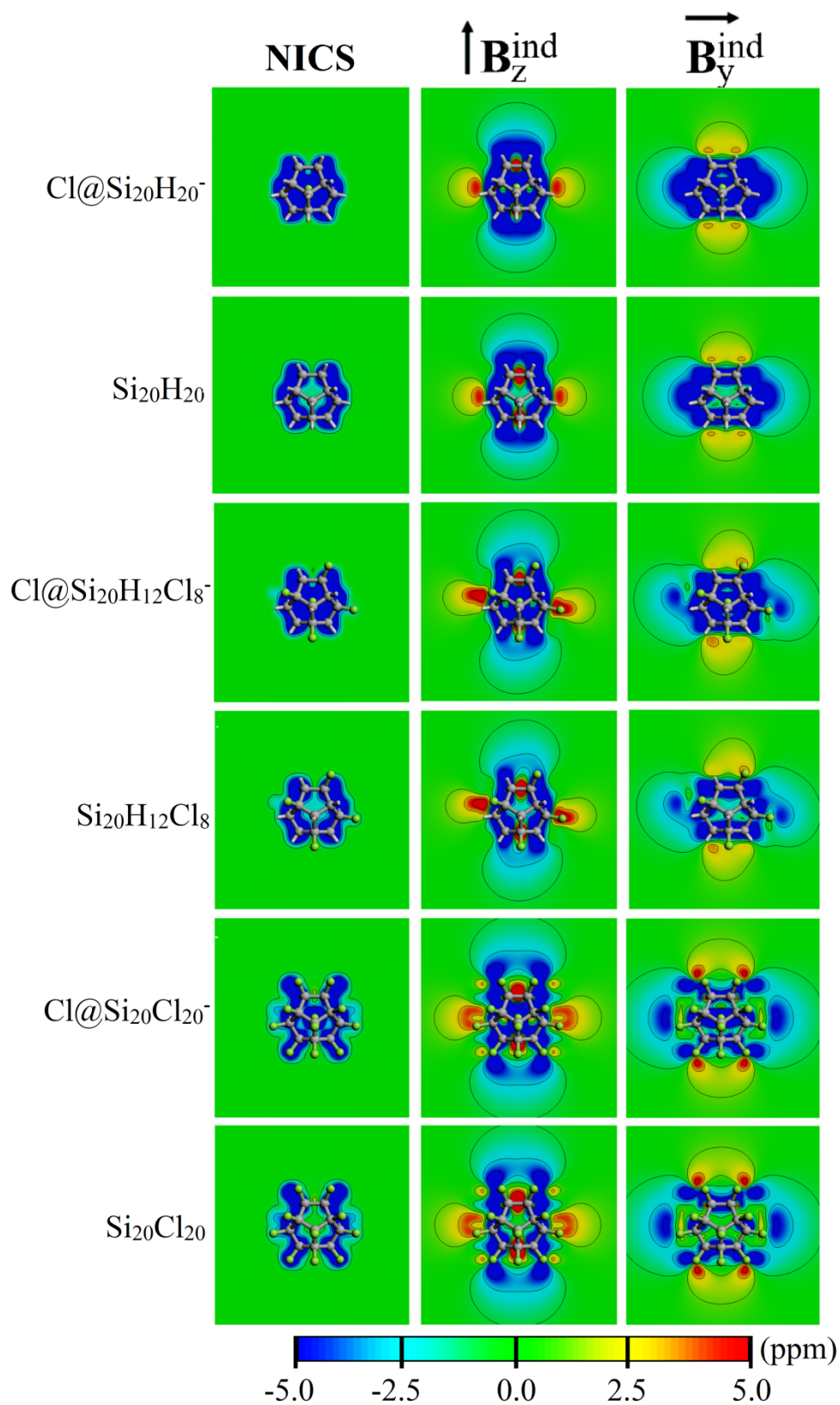


Figure S1. Contour plot representation of NICS, z- and y-component of the induced magnetic field,  $B_z^{\text{ind}}$  and  $B_y^{\text{ind}}$ , for  $\text{Si}_{20}\text{H}_{20}$ ,  $\text{Si}_{20}\text{H}_{12}\text{Cl}_8$ , and,  $\text{Si}_{20}\text{Cl}_{20}$ . In addition, **1**, **2** and **3**, are given for comparison.

Table S1. Coordinates for optimized structures in multiXYZ format. In Angstrom ( $\text{\AA}$ ) units.

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40
Si20Cl20 q=0
Si      8.678952000      6.870952000      9.046233000
Si     10.552893000      8.301862000      8.921550000
Si      9.789216000     10.522049000      9.152767000
Si      7.448785000     10.442563000      9.396005000
Si      6.758753000      8.193790000      9.341795000
Si      5.801152000      7.675218000     11.432651000
Si      7.138036000      6.004282000     12.439071000
Si      8.919641000      5.517783000     10.957017000
Si     10.913740000      6.104336000     12.053708000
Si     11.932360000      7.822510000     10.783073000
Cl      8.497720000      5.701680000      7.364780000
Cl     11.548296000      8.047370000      7.128142000
Cl     10.298734000     11.681036000      7.521754000
Cl      6.516679000     11.486157000      7.886139000
Cl      5.398294000      7.872014000      7.837821000
Cl      3.836179000      7.112022000     11.176685000
Cl      6.068089000      4.288375000     12.875815000
Cl      8.984799000      3.538144000     10.376970000
Cl     12.114306000      4.445602000     12.269370000
Cl     13.842477000      7.279360000     10.202320000
Si      9.153742000     10.560048000     14.523327000
Si      7.279800000      9.129138000     14.648010000
Si      8.043477000      6.908951000     14.416792000
Si     10.383908000      6.988437000     14.173555000
Si     11.073941000      9.237210000     14.227765000
Si     12.031542000      9.755782000     12.136909000
Si     10.694658000     11.426718000     11.130489000
Si      8.913052000     11.913217000     12.612543000
Si      6.918953000     11.326664000     11.515851000
Si      5.900334000      9.608490000     12.786486000
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Cl      5.718387000     12.985398000     11.300190000
Cl      3.990217000     10.151640000     13.367240000
41
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Cl      8.916347000      8.715500000     11.784780000
Si      8.678952000      6.870952000      9.046233000
Si     10.552893000      8.301862000      8.921550000
Si      9.789216000     10.522049000      9.152767000
Si      7.448785000     10.442563000      9.396005000
Si      6.758753000      8.193790000      9.341795000
Si      5.801152000      7.675218000     11.432651000
Si      7.138036000      6.004282000     12.439071000
Si      8.919641000      5.517783000     10.957017000
Si     10.913740000      6.104336000     12.053708000
Si     11.932360000      7.822510000     10.783073000
Cl      8.497720000      5.701680000      7.364780000
Cl     11.548296000      8.047370000      7.128142000
Cl     10.298734000     11.681036000      7.521754000
Cl      6.516679000     11.486157000      7.886139000
Cl      5.398294000      7.872014000      7.837821000
Cl      3.836179000      7.112022000     11.176685000

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Cl	6.068089000	4.288375000	12.875815000
Cl	8.984799000	3.538144000	10.376970000
Cl	12.114306000	4.445602000	12.269370000
Cl	13.842477000	7.279360000	10.202320000
Si	9.153742000	10.560048000	14.523327000
Si	7.279800000	9.129138000	14.648010000
Si	8.043477000	6.908951000	14.416792000
Si	10.383908000	6.988437000	14.173555000
Si	11.073941000	9.237210000	14.227765000
Si	12.031542000	9.755782000	12.136909000
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Si	8.913052000	11.913217000	12.612543000
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Cl	5.718387000	12.985398000	11.300190000
Cl	3.990217000	10.151640000	13.367240000
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Si	9.182919000	12.482547000	3.785238000
H	8.275362000	11.822874000	2.789733000
Si	11.395840000	12.616741000	2.999665000
Si	12.113708000	14.858035000	2.943950000
H	12.478826000	15.289438000	1.554566000
Si	11.037363000	17.159641000	5.776026000
H	10.955978000	18.653158000	5.663371000
Si	8.195927000	14.808453000	6.605279000
Si	9.262814000	11.294509000	5.827060000
Si	12.801816000	11.385700000	4.420160000
H	13.513785000	10.279031000	3.700084000
Si	13.932386000	15.064637000	4.426845000
H	15.158742000	15.595385000	3.745547000
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H	8.990750000	17.471548000	8.249301000
Si	8.571890000	12.694604000	7.576270000
H	7.345113000	12.168776000	8.260756000
Si	11.458928000	10.593472000	6.167587000
H	11.537721000	9.099262000	6.273199000
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Si	13.979606000	13.063820000	7.705528000
H	15.215313000	12.663893000	8.455934000
Si	13.310248000	15.255309000	8.232141000
H	14.218005000	15.900263000	9.237118000
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41			
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Si	9.182919000	12.482547000	3.785238000
H	8.275362000	11.822874000	2.789733000
Si	11.395840000	12.616741000	2.999665000
Si	12.113708000	14.858035000	2.943950000
H	12.478826000	15.289438000	1.554566000
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Si	9.262814000	11.294509000	5.827060000
Si	12.801816000	11.385700000	4.420160000
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H	15.158742000	15.595385000	3.745547000
Si	9.702096000	16.359640000	7.536825000
H	8.990750000	17.471548000	8.249301000
Si	8.571890000	12.694604000	7.576270000
H	7.345113000	12.168776000	8.260756000
Si	11.458928000	10.593472000	6.167587000
H	11.537721000	9.099262000	6.273199000
Si	14.295168000	12.942823000	5.375551000
Si	13.230955000	16.453724000	6.201684000
Si	11.085814000	15.123354000	8.995205000
Si	10.393321000	12.871087000	9.056937000
H	10.037880000	12.427231000	10.444939000
Si	12.182533000	11.620248000	8.153918000
Si	13.979606000	13.063820000	7.705528000
H	15.215313000	12.663893000	8.455934000
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H	14.218005000	15.900263000	9.237118000
Cl	9.720710000	17.624054000	2.460126000
Cl	11.466983000	11.836914000	1.047208000
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Cl	10.888667000	15.930070000	10.936296000
Cl	12.845367000	10.090070000	9.420641000
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H	-2.254735000	8.577530000	3.793876000
Si	-0.039048000	6.414871000	3.137229000
H	0.473614000	6.579104000	4.426189000
Si	-0.724869000	4.206607000	2.680048000
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Si	1.009082000	8.691121000	0.279942000
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H	2.771793000	7.264121000	2.529251000
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H	3.348193000	4.422422000	0.498186000
Si	0.593067000	3.381353000	0.922218000
H	1.282016000	2.197462000	1.245464000
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H	-0.812362000	1.599893000	-1.264625000
Si	-3.016470000	3.544505000	-0.279942000
H	-3.837301000	2.417060000	-0.344898000
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H	-4.779182000	4.971505000	-2.529251000
Si	-4.127464000	7.171465000	-0.289523000
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Si	-2.600455000	8.854274000	-0.922218000
H	-3.289405000	10.038164000	-1.245464000
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H	-2.254735000	8.577530000	3.793876000
Si	-0.039048000	6.414871000	3.137229000
H	0.473614000	6.579104000	4.426189000
Si	-0.724869000	4.206607000	2.680048000
H	-0.657798000	3.301004000	3.736393000
Si	-2.965796000	4.295049000	1.949056000
H	-3.819652000	3.534994000	2.740021000
Si	-3.637288000	6.557161000	1.935452000
H	-4.753991000	6.737640000	2.759182000
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Si	-1.282519000	8.029020000	-2.680048000
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Si	-4.127464000	7.171465000	-0.289523000
H	-5.355582000	7.813204000	-0.498186000
Si	-2.600455000	8.854274000	-0.922218000
H	-3.289405000	10.038164000	-1.245464000