Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Local and Global Aromaticity under Rotation. Analysis of Two- and Three-Dimensional Representative Carbon Nanostructures

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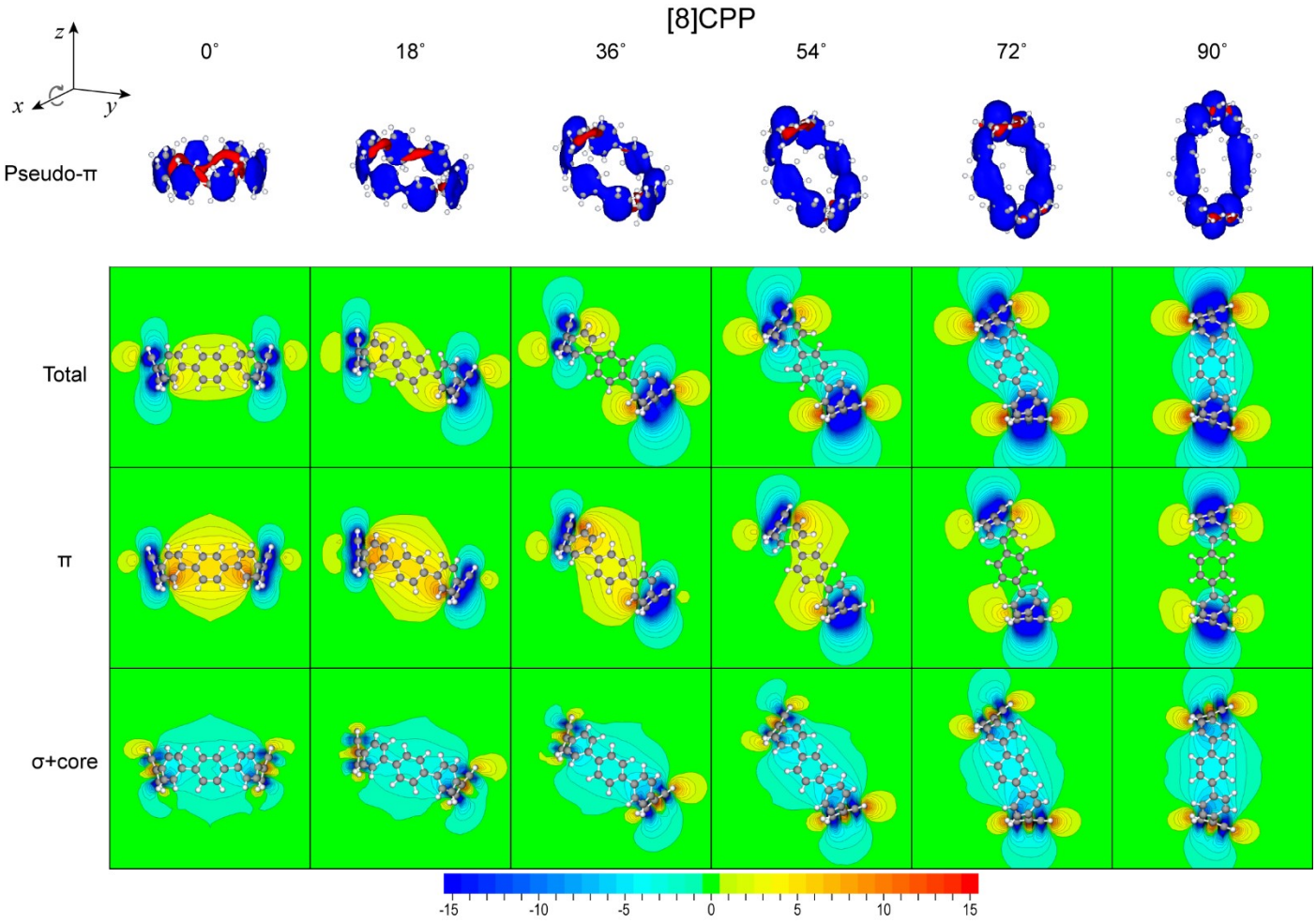


Figure S1. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind}, and 3D isosurfaces (5ppm) of pseudo-π contributions, of [8]CPP at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.

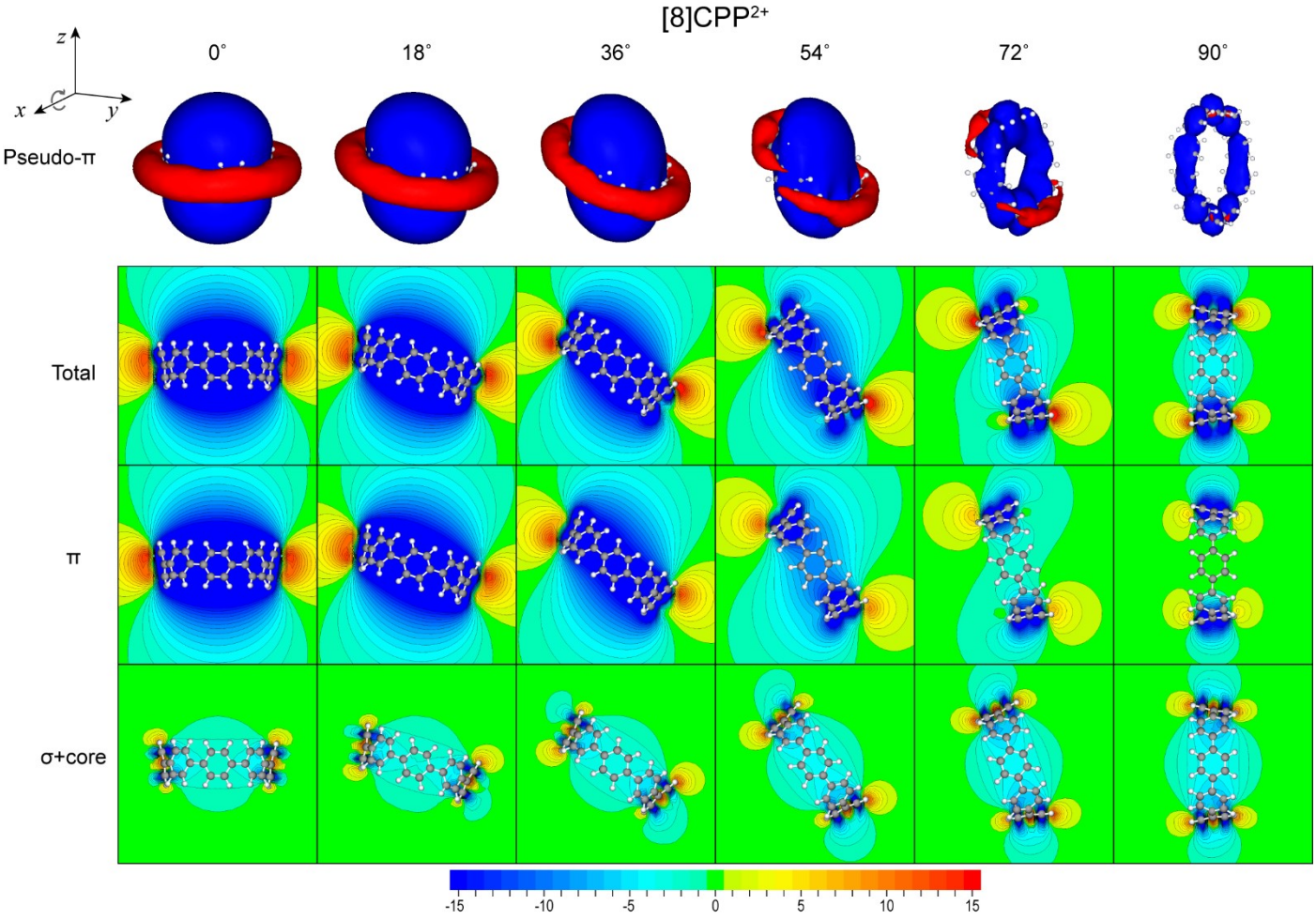


Figure S2. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind}, and 3D isosurfaces (5ppm) of pseudo-π contributions, of [8]CPP^{2+} at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.

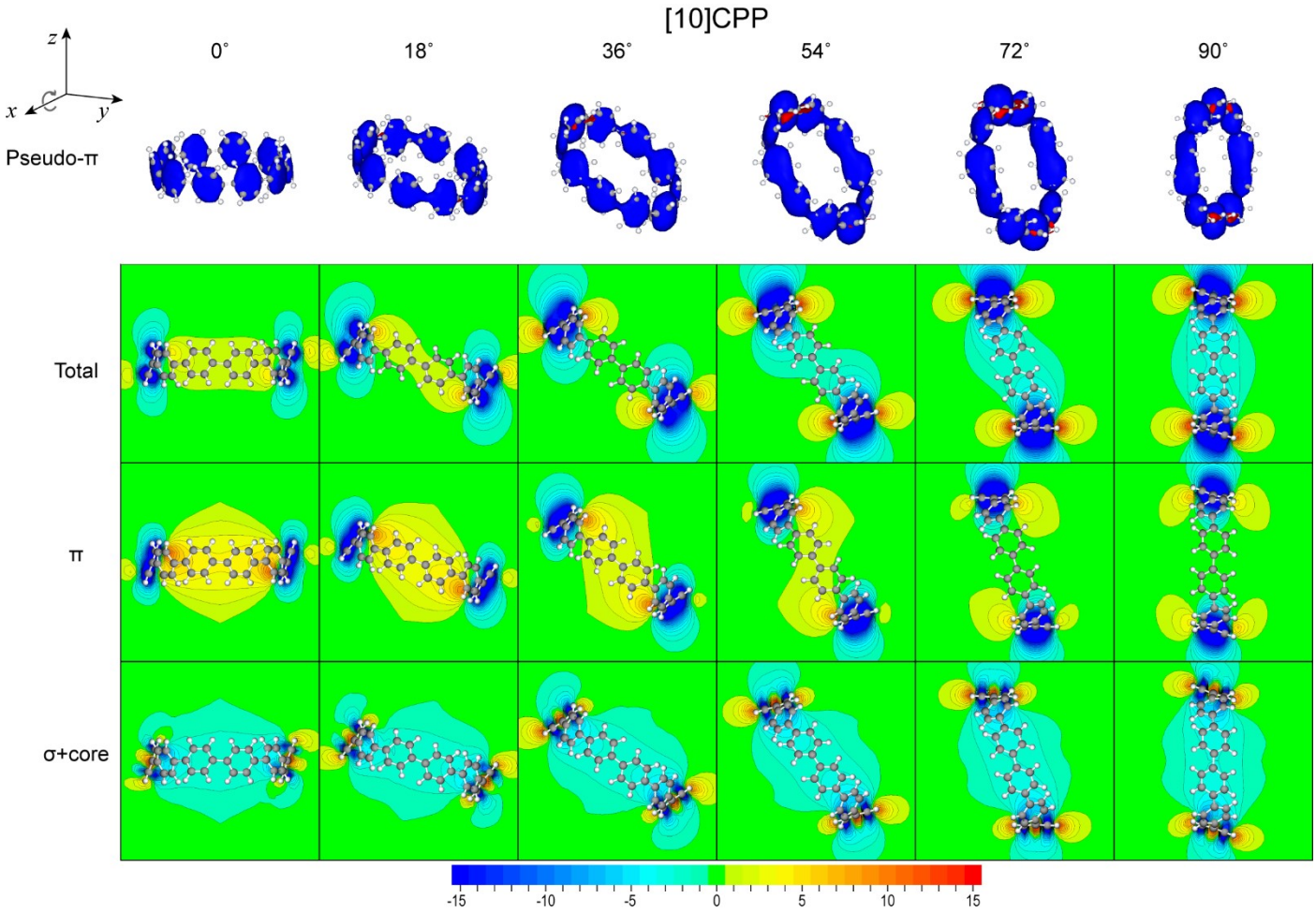


Figure S3. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind}, and 3D isosurfaces (5ppm) of pseudo-π contributions, of [10]CPP at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.

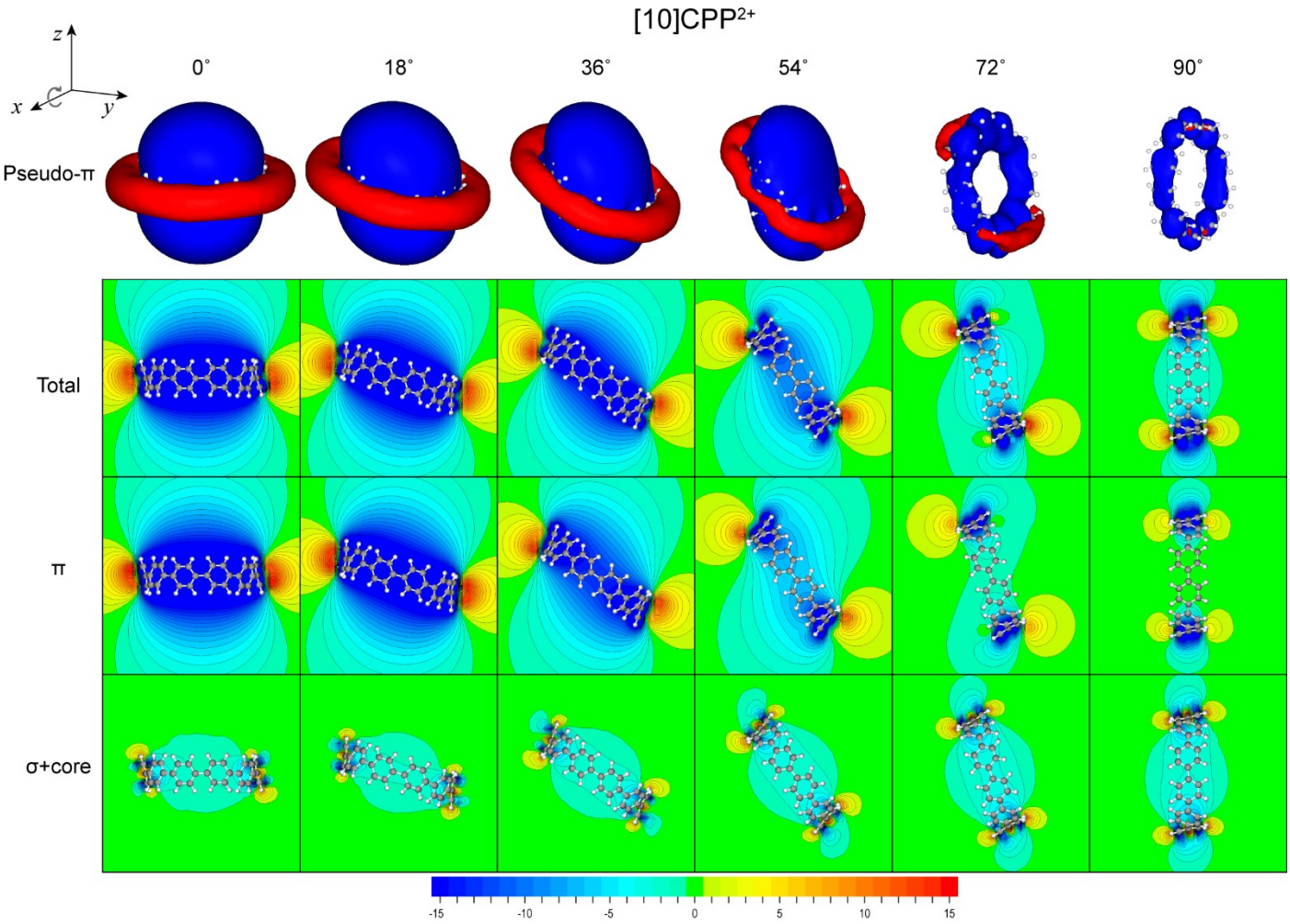


Figure S4. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind}, and 3D isosurfaces (5ppm) of pseudo-π contributions, of [10]CPP^{2+} at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.

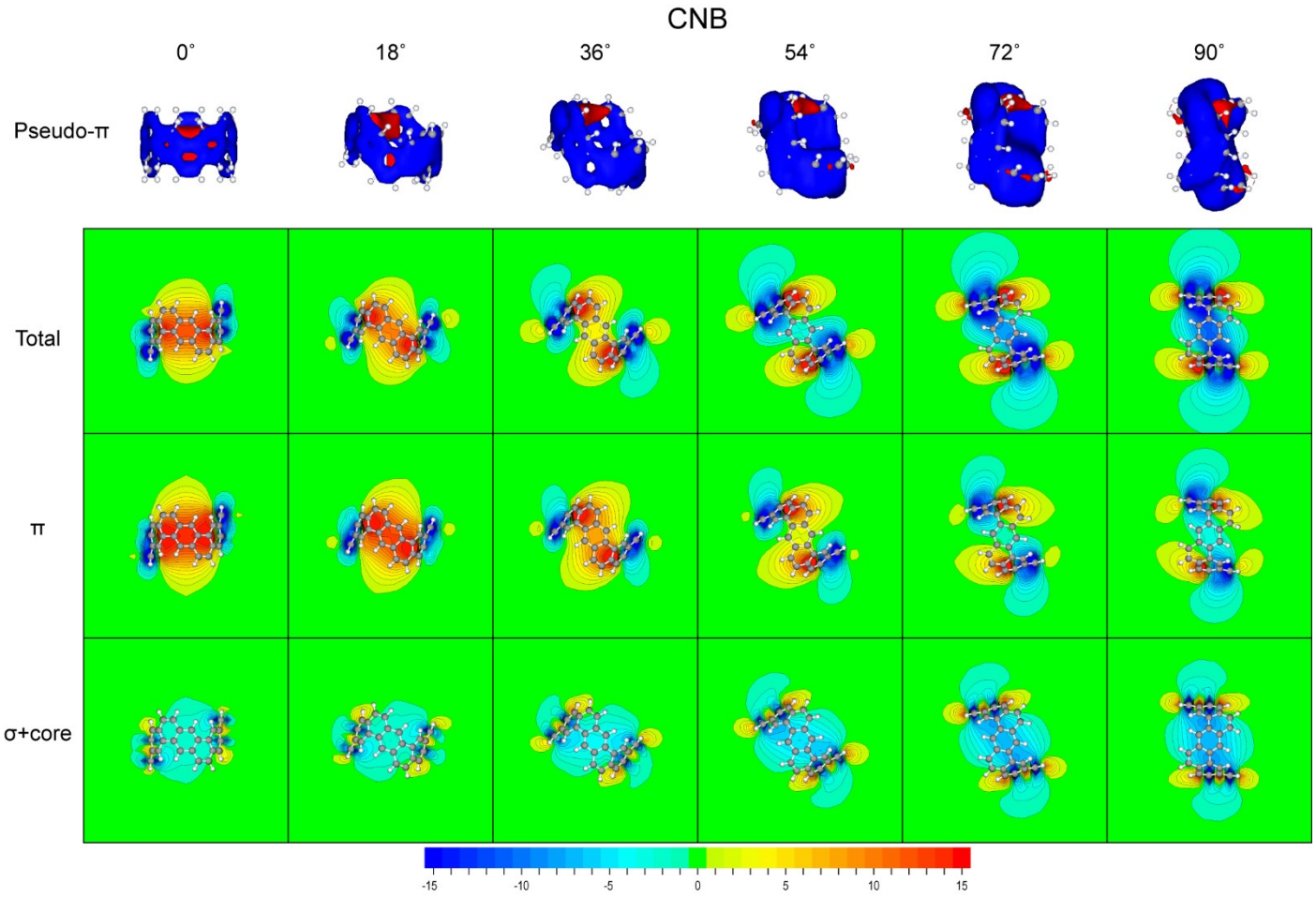


Figure S5. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind}, and 3D isosurfaces (5ppm) of pseudo-π contributions, of CNB at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.

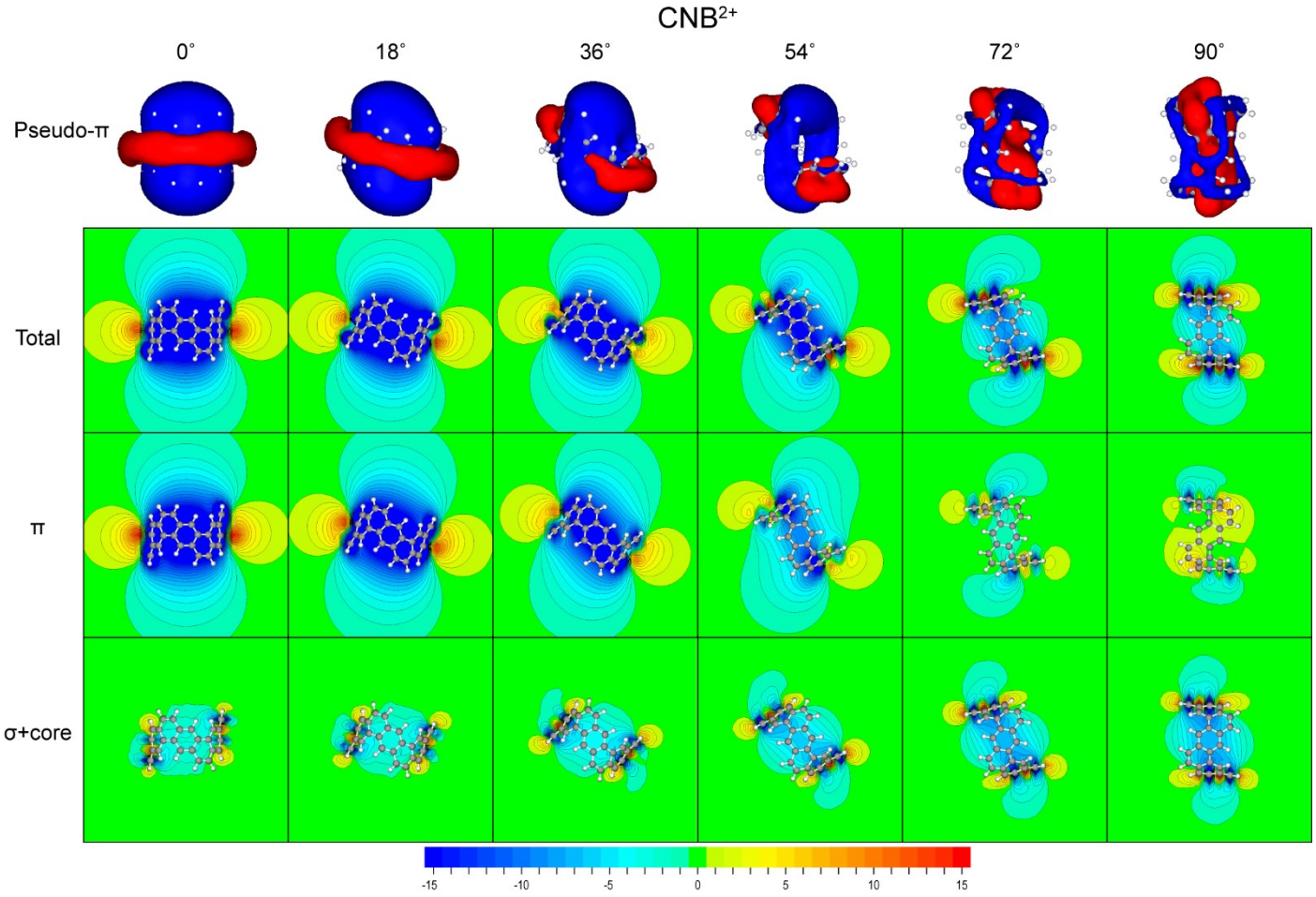
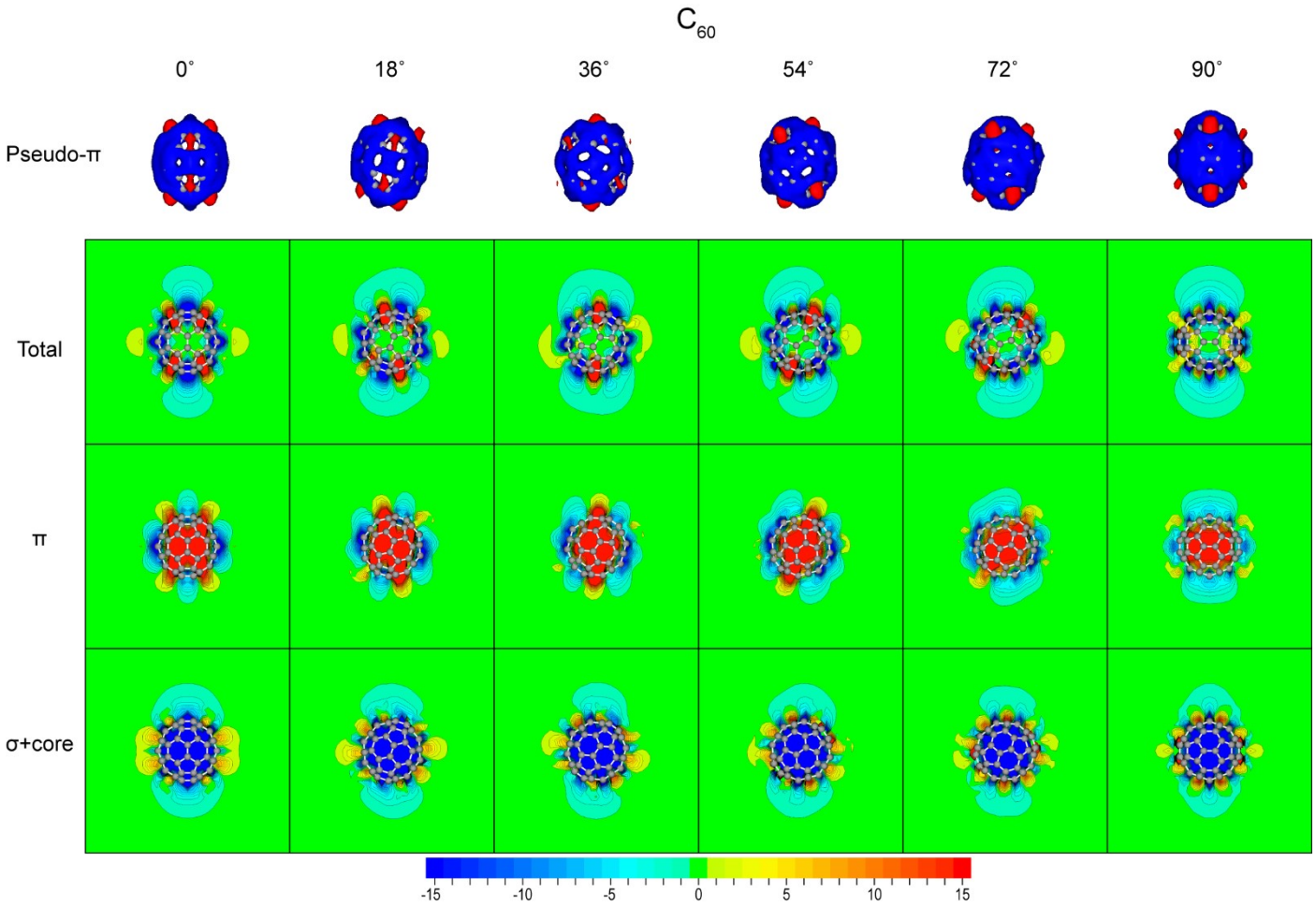


Figure S6. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind} , and 3D isosurfaces (5ppm) of pseudo-π contributions, of CNB^{2+} at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.



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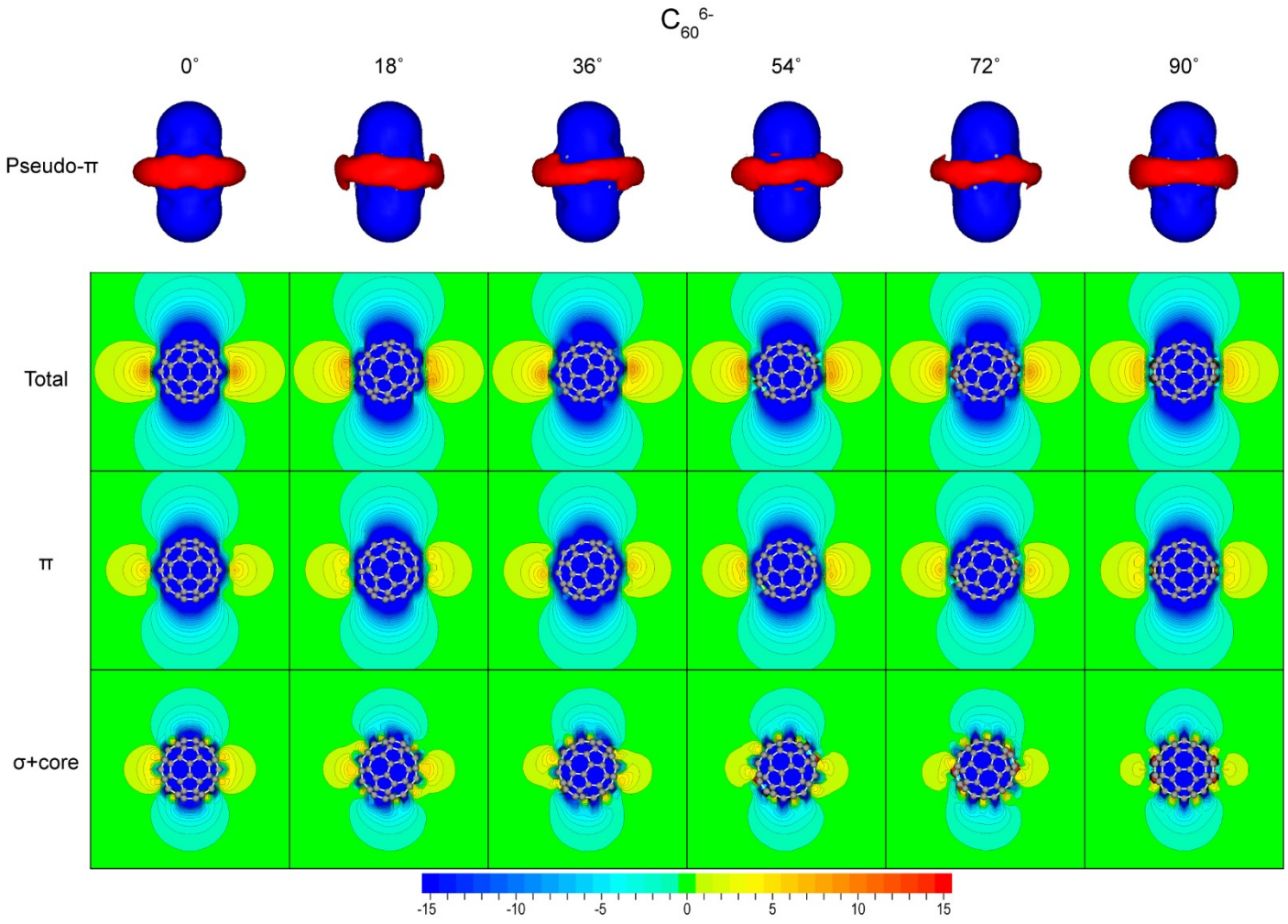

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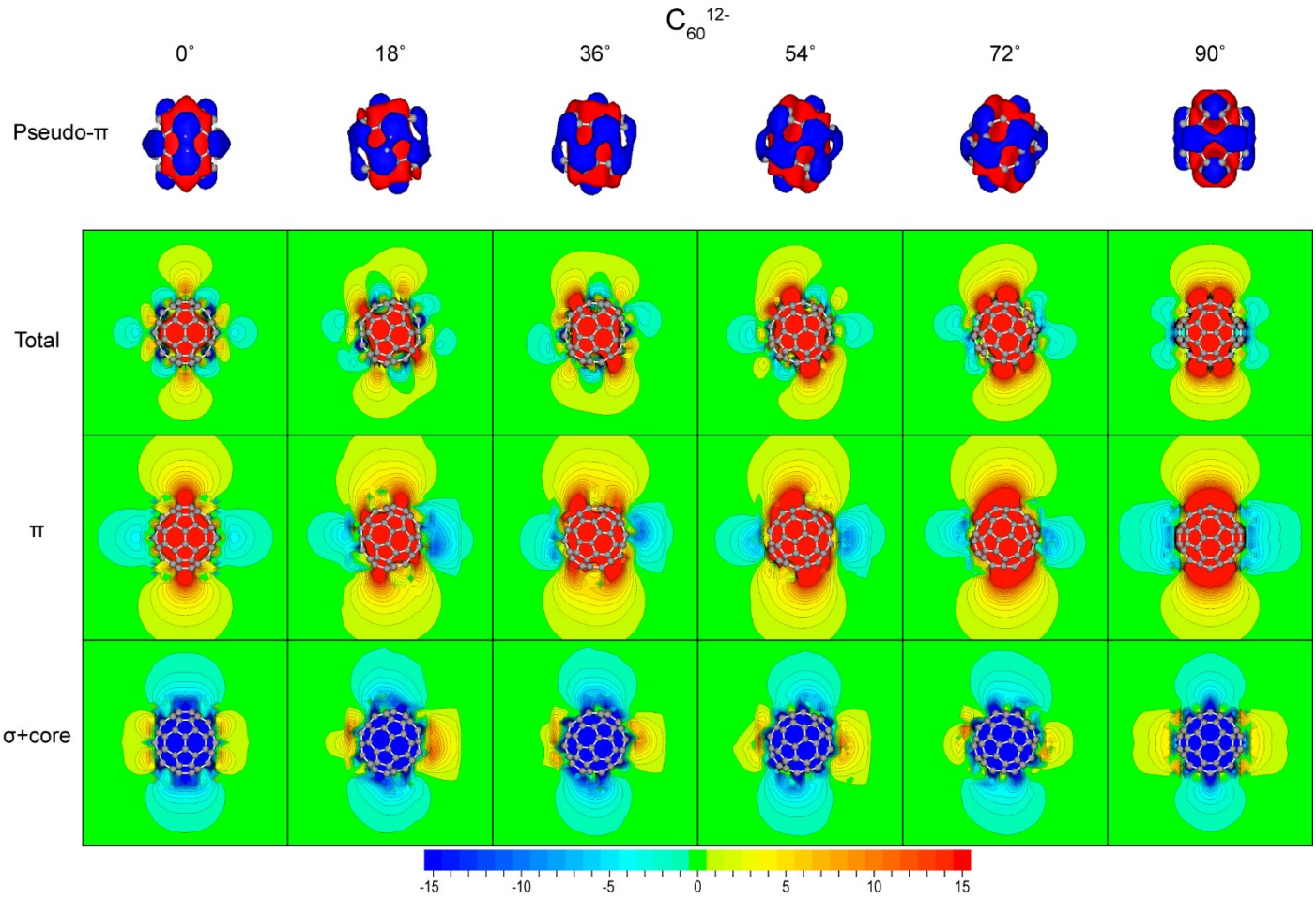

Figure S9. Contour maps of total and π, σ+core contributions to the z component of the induced magnetic field, B_z^{ind} , and 3D isosurfaces (5ppm) of pseudo-π contributions, of C_{60}^{12-} at tilt angles of 0°, 18°, 36°, 54°, 72° and 90°.

Table S1. Central Nucleus-Independent Chemical Shift tensor for the studied species calculated at the PBE/TZ2P level, which remain under rotation, as given by their principal-axis-system (PAS) for the shielding tensor (σ), denoting the average, the NICS(0) value NICS(0) = $-1/3*(\sigma_{11}+\sigma_{22}+\sigma_{33})$ and the anisotropic term $NICS_{aniso} = -(\sigma_{33}-1/2*(\sigma_{11}+\sigma_{22}))$. Values are given in ppm.

	PAS components					
	σ_{11}	σ_{22}	σ_{33}	Average	NICS(0)	$NICS_{Aniso}$
[10]CPP	-1.6	3.1	3.1	1.6	-1.6	-2.4
$[10]CPP^{2+}$	2.7	2.7	25.9	10.4	-10.4	-23.2
[8]CPP	-2.7	4.7	4.7	2.2	-2.2	-3.7
$[8]CPP^{2+}$	4.4	4.4	31.9	13.5	-13.5	-27.5
CNB	-11.6	11.5	11.5	3.8	-3.8	-11.5
CNB^{2+}	7.0	7.0	35.3	16.4	-16.4	-28.3
C_{60}	1.0	1.0	1.0	1.0	-1.0	0.0
C_{60}^{6-}	51.8	51.8	51.8	51.8	-51.8	0.0
C_{60}^{12-}	-35.8	-35.8	-35.8	-35.8	35.8	0.0