

Supplementary Information

Optical Properties of Bimetallic Compositional Heterodimers

Junais Habeeb Mokkath

j.mokath@kcst.edu.kw

Department of Physics, Kuwait College of Science And Technology, Doha Area, 7th Ring Road, P.O.
Box 27235, Kuwait

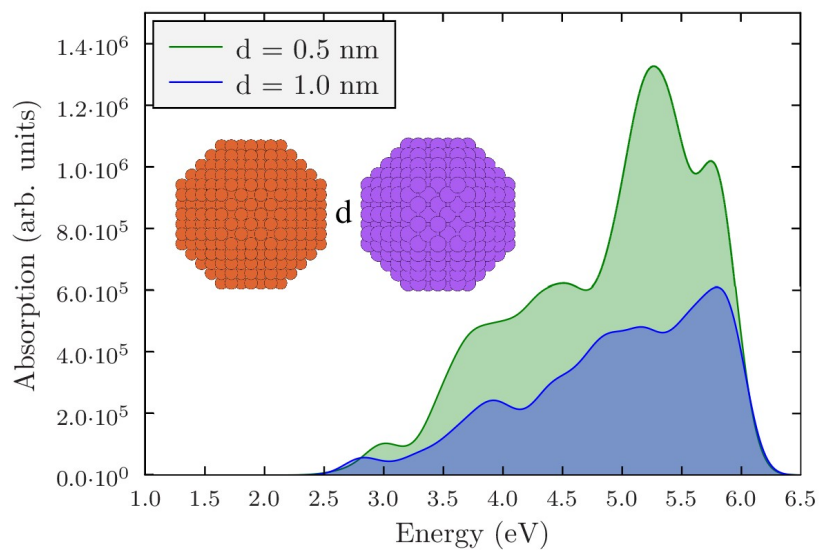


Figure S1: TDDFT calculated absorption spectra of **Li 1.50 nm and Na 1.50 nm heterodimer** as a function of different d values.

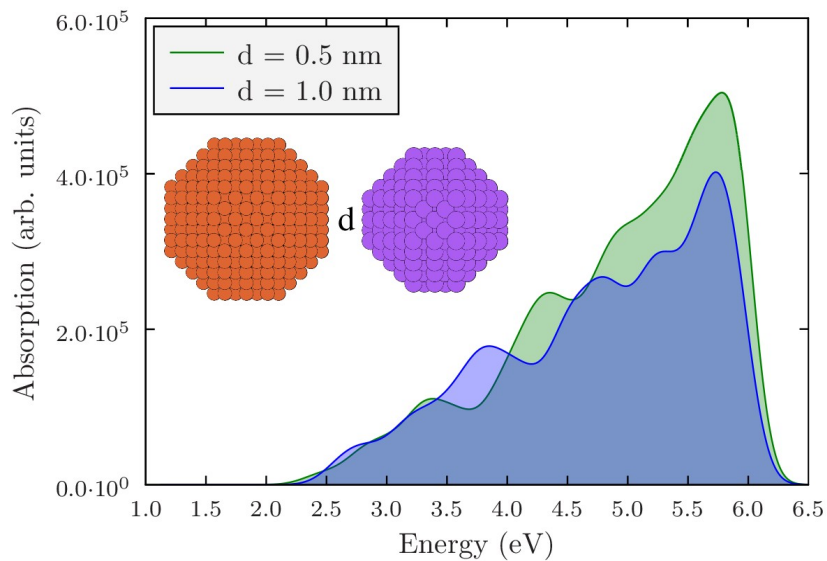


Figure S2: TDDFT calculated absorption spectra of **Li 1.50 nm and Na 1.25 nm heterodimer** as a function of different d values.

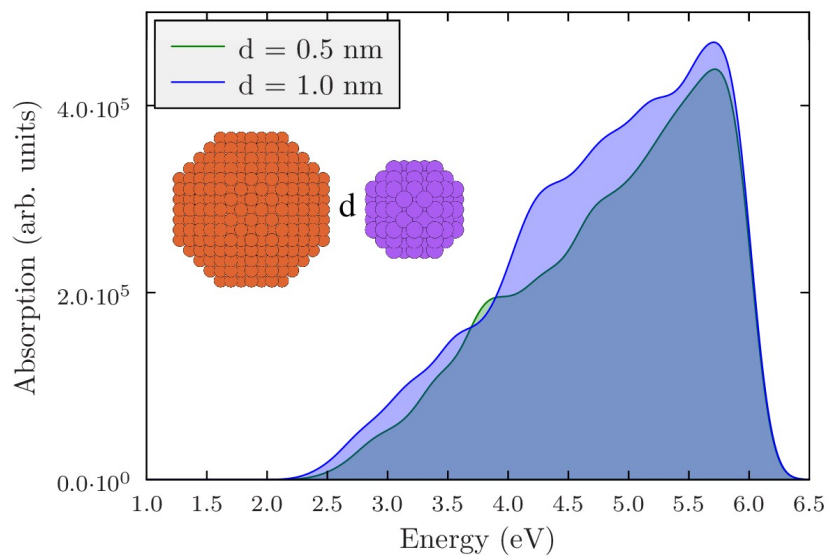


Figure S3: TDDFT calculated absorption spectra of **Li 1.50 nm and Na 1.0 nm heterodimer** as a function of different d values.

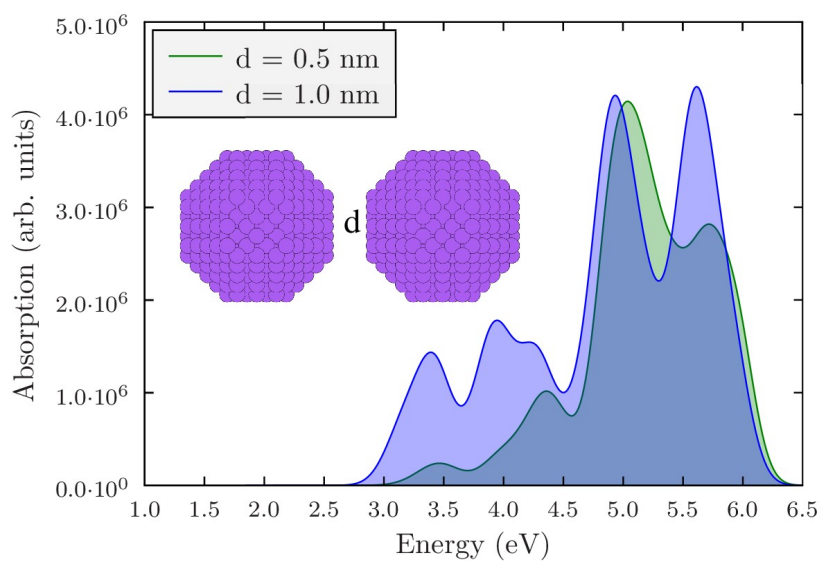


Figure S4: TDDFT calculated absorption spectra of **Na 1.50 nm and Na 1.50 nm heterodimer** as a function of different d values.

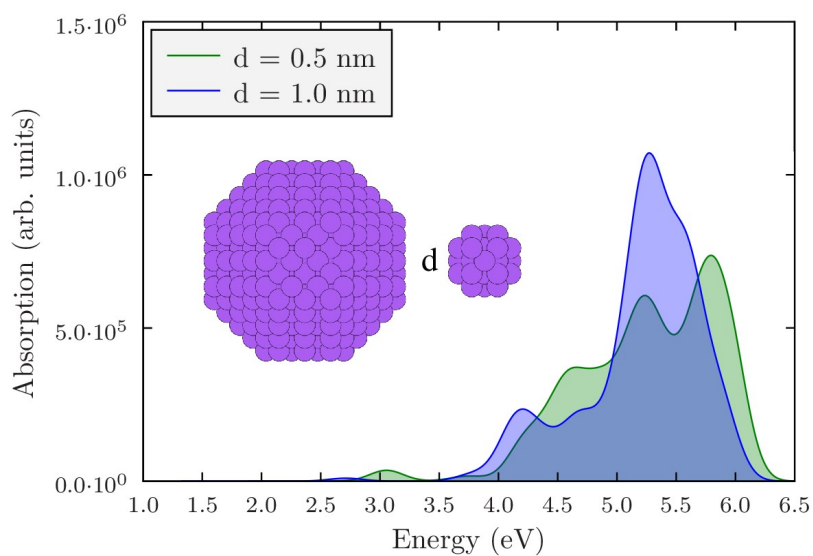


Figure S5: TDDFT calculated absorption spectra of **Na 1.50 nm and Na 0.50 nm heterodimer** as a function of different d values.

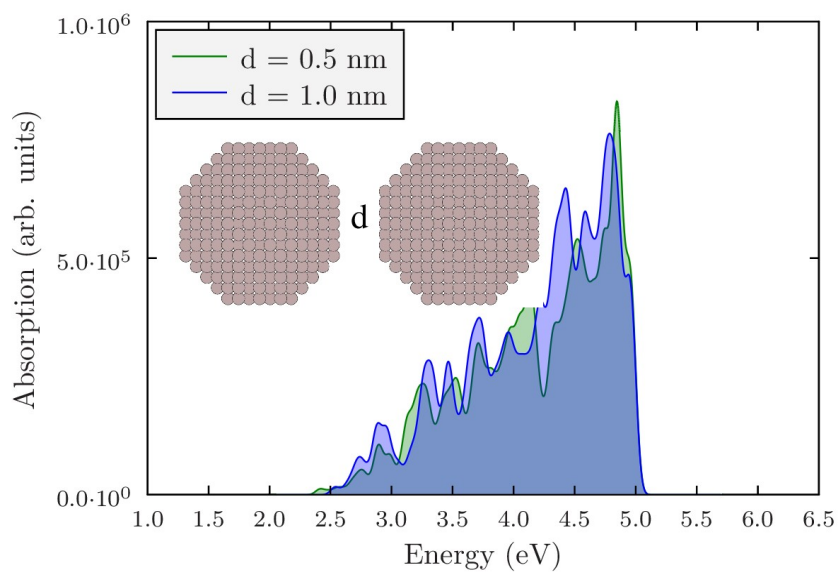


Figure S6: TDDFT calculated absorption spectra of **Al 1.50 nm and Al 1.50 nm heterodimer** as a function of different d values.

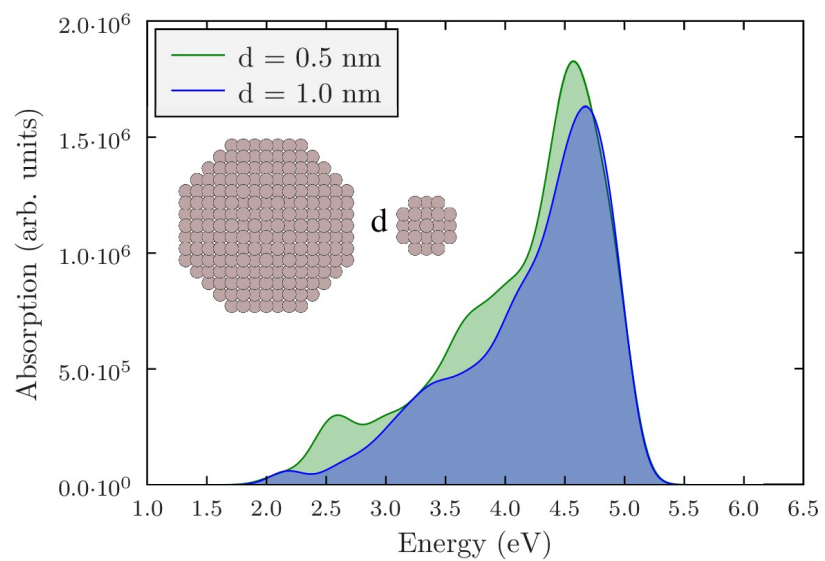


Figure S7: TDDFT calculated absorption spectra of **Al 1.50 nm and Al 0.50 nm heterodimer** as a function of different d values.

Atomic coordinates of Na 1.50 nm nanoparticle

Na	2.822311e+01	1.809916e+01	1.000000e+01
Na	3.024790e+01	2.012395e+01	1.000000e+01
Na	2.822311e+01	1.607437e+01	1.202479e+01
Na	3.024790e+01	1.809916e+01	1.202479e+01
Na	3.227269e+01	2.012395e+01	1.202479e+01
Na	2.822311e+01	1.404958e+01	1.404958e+01
Na	3.024790e+01	1.607437e+01	1.404958e+01
Na	3.227269e+01	1.809916e+01	1.404958e+01
Na	3.429748e+01	2.012395e+01	1.404958e+01
Na	2.822311e+01	1.202479e+01	1.607437e+01
Na	3.024790e+01	1.404958e+01	1.607437e+01
Na	3.227269e+01	1.607437e+01	1.607437e+01
Na	3.429748e+01	1.809916e+01	1.607437e+01
Na	3.632227e+01	2.012395e+01	1.607437e+01
Na	2.822311e+01	1.000000e+01	1.809916e+01
Na	3.024790e+01	1.202479e+01	1.809916e+01
Na	3.227269e+01	1.404958e+01	1.809916e+01
Na	3.429748e+01	1.607437e+01	1.809916e+01
Na	3.632227e+01	1.809916e+01	1.809916e+01
Na	3.834706e+01	2.012395e+01	1.809916e+01
Na	3.024790e+01	1.000000e+01	2.012395e+01
Na	3.227269e+01	1.202479e+01	2.012395e+01
Na	3.429748e+01	1.404958e+01	2.012395e+01
Na	3.632227e+01	1.607437e+01	2.012395e+01
Na	3.834706e+01	1.809916e+01	2.012395e+01
Na	2.417353e+01	1.809916e+01	1.000000e+01
Na	2.619832e+01	2.012395e+01	1.000000e+01
Na	2.822311e+01	2.214874e+01	1.000000e+01
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Na 2.417353e+01 2.822311e+01 3.632227e+01
Na 2.619832e+01 3.024790e+01 3.632227e+01
Na 2.822311e+01 3.227269e+01 3.632227e+01
Na 1.809916e+01 2.012395e+01 3.834706e+01
Na 2.012395e+01 2.214874e+01 3.834706e+01
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Na 2.417353e+01 2.619832e+01 3.834706e+01
Na 2.619832e+01 2.822311e+01 3.834706e+01
Na 2.822311e+01 3.024790e+01 3.834706e+01
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Na 1.202479e+01 3.227269e+01 2.417353e+01
Na 1.404958e+01 3.429748e+01 2.417353e+01
Na 1.607437e+01 3.632227e+01 2.417353e+01
Na 1.809916e+01 3.834706e+01 2.417353e+01
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Atomic coordinates of Na 1.25 nm nanoparticle

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Na 6.074370e+00 -6.074370e+00 -8.099160e+00
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Na 6.074370e+00 -8.099160e+00 -6.074370e+00
Na 8.099160e+00 -6.074370e+00 -6.074370e+00

Na 1.012395e+01 -4.049580e+00 -6.074370e+00
Na 4.049580e+00 -1.214874e+01 -4.049580e+00
Na 6.074370e+00 -1.012395e+01 -4.049580e+00
Na 8.099160e+00 -8.099160e+00 -4.049580e+00
Na 1.012395e+01 -6.074370e+00 -4.049580e+00
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Na 0.000000e+00 -4.049580e+00 -1.214874e+01
Na 2.024790e+00 -2.024790e+00 -1.214874e+01
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Na -2.024790e+00 8.099160e+00 6.074370e+00
Na 0.000000e+00 1.012395e+01 6.074370e+00
Na -8.099160e+00 -0.000000e+00 8.099160e+00
Na -6.074370e+00 2.024790e+00 8.099160e+00
Na -4.049580e+00 4.049580e+00 8.099160e+00
Na -2.024790e+00 6.074370e+00 8.099160e+00
Na 0.000000e+00 8.099160e+00 8.099160e+00
Na -6.074370e+00 -0.000000e+00 1.012395e+01
Na -4.049580e+00 2.024790e+00 1.012395e+01
Na -2.024790e+00 4.049580e+00 1.012395e+01
Na 0.000000e+00 6.074370e+00 1.012395e+01
Na -4.049580e+00 -0.000000e+00 1.214874e+01
Na -2.024790e+00 2.024790e+00 1.214874e+01
Na 0.000000e+00 4.049580e+00 1.214874e+01
Na -1.214874e+01 4.049580e+00 4.049580e+00
Na -1.012395e+01 6.074370e+00 4.049580e+00
Na -8.099160e+00 8.099160e+00 4.049580e+00
Na -6.074370e+00 1.012395e+01 4.049580e+00
Na -4.049580e+00 1.214874e+01 4.049580e+00
Na -1.012395e+01 4.049580e+00 6.074370e+00

Na -8.099160e+00 6.074370e+00 6.074370e+00
Na -6.074370e+00 8.099160e+00 6.074370e+00
Na -4.049580e+00 1.012395e+01 6.074370e+00
Na -8.099160e+00 4.049580e+00 8.099160e+00
Na -6.074370e+00 6.074370e+00 8.099160e+00
Na -4.049580e+00 8.099160e+00 8.099160e+00
Na -6.074370e+00 4.049580e+00 1.012395e+01
Na -4.049580e+00 6.074370e+00 1.012395e+01
Na -4.049580e+00 4.049580e+00 1.214874e+01

Atomic coordinates of Na 1.00 nm nanoparticle

Na 4.049580e+00 -4.049580e+00 -8.099160e+00
Na 4.049580e+00 -6.074370e+00 -6.074370e+00
Na 6.074370e+00 -4.049580e+00 -6.074370e+00
Na 4.049580e+00 -8.099160e+00 -4.049580e+00
Na 6.074370e+00 -6.074370e+00 -4.049580e+00
Na 8.099160e+00 -4.049580e+00 -4.049580e+00
Na 0.000000e+00 -4.049580e+00 -8.099160e+00
Na 2.024790e+00 -2.024790e+00 -8.099160e+00
Na 4.049580e+00 0.000000e+00 -8.099160e+00
Na 0.000000e+00 -6.074370e+00 -6.074370e+00
Na 2.024790e+00 -4.049580e+00 -6.074370e+00
Na 4.049580e+00 -2.024790e+00 -6.074370e+00
Na 6.074370e+00 0.000000e+00 -6.074370e+00
Na 0.000000e+00 -8.099160e+00 -4.049580e+00
Na 2.024790e+00 -6.074370e+00 -4.049580e+00
Na 4.049580e+00 -4.049580e+00 -4.049580e+00
Na 6.074370e+00 -2.024790e+00 -4.049580e+00
Na 8.099160e+00 0.000000e+00 -4.049580e+00
Na 2.024790e+00 -8.099160e+00 -2.024790e+00
Na 4.049580e+00 -6.074370e+00 -2.024790e+00

Na 6.074370e+00 -4.049580e+00 -2.024790e+00
Na 8.099160e+00 -2.024790e+00 -2.024790e+00
Na 4.049580e+00 -8.099160e+00 0.000000e+00
Na 6.074370e+00 -6.074370e+00 0.000000e+00
Na 8.099160e+00 -4.049580e+00 0.000000e+00
Na -4.049580e+00 -4.049580e+00 -8.099160e+00
Na -2.024790e+00 -2.024790e+00 -8.099160e+00
Na 0.000000e+00 0.000000e+00 -8.099160e+00
Na 2.024790e+00 2.024790e+00 -8.099160e+00
Na 4.049580e+00 4.049580e+00 -8.099160e+00
Na -4.049580e+00 -6.074370e+00 -6.074370e+00
Na -2.024790e+00 -4.049580e+00 -6.074370e+00
Na 0.000000e+00 -2.024790e+00 -6.074370e+00
Na 2.024790e+00 0.000000e+00 -6.074370e+00
Na 4.049580e+00 2.024790e+00 -6.074370e+00
Na 6.074370e+00 4.049580e+00 -6.074370e+00
Na -4.049580e+00 -8.099160e+00 -4.049580e+00
Na -2.024790e+00 -6.074370e+00 -4.049580e+00
Na 0.000000e+00 -4.049580e+00 -4.049580e+00
Na 2.024790e+00 -2.024790e+00 -4.049580e+00
Na 4.049580e+00 0.000000e+00 -4.049580e+00
Na 6.074370e+00 2.024790e+00 -4.049580e+00
Na 8.099160e+00 4.049580e+00 -4.049580e+00
Na -2.024790e+00 -8.099160e+00 -2.024790e+00
Na 0.000000e+00 -6.074370e+00 -2.024790e+00
Na 2.024790e+00 -4.049580e+00 -2.024790e+00
Na 4.049580e+00 -2.024790e+00 -2.024790e+00
Na 6.074370e+00 0.000000e+00 -2.024790e+00
Na 8.099160e+00 2.024790e+00 -2.024790e+00
Na 0.000000e+00 -8.099160e+00 0.000000e+00
Na 2.024790e+00 -6.074370e+00 0.000000e+00
Na 4.049580e+00 -4.049580e+00 0.000000e+00
Na 6.074370e+00 -2.024790e+00 0.000000e+00

Na 8.099160e+00 0.000000e+00 0.000000e+00
Na 2.024790e+00 -8.099160e+00 2.024790e+00
Na 4.049580e+00 -6.074370e+00 2.024790e+00
Na 6.074370e+00 -4.049580e+00 2.024790e+00
Na 8.099160e+00 -2.024790e+00 2.024790e+00
Na 4.049580e+00 -8.099160e+00 4.049580e+00
Na 6.074370e+00 -6.074370e+00 4.049580e+00
Na 8.099160e+00 -4.049580e+00 4.049580e+00
Na -4.049580e+00 0.000000e+00 -8.099160e+00
Na -2.024790e+00 2.024790e+00 -8.099160e+00
Na 0.000000e+00 4.049580e+00 -8.099160e+00
Na -6.074370e+00 -4.049580e+00 -6.074370e+00
Na -4.049580e+00 -2.024790e+00 -6.074370e+00
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Na -2.024790e+00 -2.024790e+00 -4.049580e+00
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Na 2.024790e+00 2.024790e+00 -4.049580e+00
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Na 6.074370e+00 6.074370e+00 -4.049580e+00
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Na 0.000000e+00 -2.024790e+00 -2.024790e+00
Na 2.024790e+00 0.000000e+00 -2.024790e+00
Na 4.049580e+00 2.024790e+00 -2.024790e+00
Na 6.074370e+00 4.049580e+00 -2.024790e+00
Na -4.049580e+00 -8.099160e+00 0.000000e+00
Na -2.024790e+00 -6.074370e+00 0.000000e+00
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Na 2.024790e+00 -2.024790e+00 0.000000e+00
Na 4.049580e+00 0.000000e+00 0.000000e+00
Na 6.074370e+00 2.024790e+00 0.000000e+00
Na 8.099160e+00 4.049580e+00 0.000000e+00
Na -2.024790e+00 -8.099160e+00 2.024790e+00
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Na 2.024790e+00 -4.049580e+00 2.024790e+00
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Na 6.074370e+00 0.000000e+00 2.024790e+00
Na 8.099160e+00 2.024790e+00 2.024790e+00
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Na 6.074370e+00 4.049580e+00 2.024790e+00
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Na 2.024790e+00 -2.024790e+00 4.049580e+00
Na 4.049580e+00 0.000000e+00 4.049580e+00
Na 6.074370e+00 2.024790e+00 4.049580e+00
Na 8.099160e+00 4.049580e+00 4.049580e+00
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Na 2.024790e+00 -4.049580e+00 6.074370e+00
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Na -8.099160e+00 0.000000e+00 -4.049580e+00
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Na -2.024790e+00 6.074370e+00 -4.049580e+00

Na 0.000000e+00 8.099160e+00 -4.049580e+00
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Na -6.074370e+00 0.000000e+00 -2.024790e+00
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Na 4.049580e+00 6.074370e+00 2.024790e+00
Na -6.074370e+00 -6.074370e+00 4.049580e+00
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Na 0.000000e+00 0.000000e+00 4.049580e+00
Na 2.024790e+00 2.024790e+00 4.049580e+00
Na 4.049580e+00 4.049580e+00 4.049580e+00
Na 6.074370e+00 6.074370e+00 4.049580e+00
Na -4.049580e+00 -6.074370e+00 6.074370e+00
Na -2.024790e+00 -4.049580e+00 6.074370e+00
Na 0.000000e+00 -2.024790e+00 6.074370e+00
Na 2.024790e+00 0.000000e+00 6.074370e+00
Na 4.049580e+00 2.024790e+00 6.074370e+00
Na 6.074370e+00 4.049580e+00 6.074370e+00

Na 0.000000e+00 -4.049580e+00 8.099160e+00
Na 2.024790e+00 -2.024790e+00 8.099160e+00
Na 4.049580e+00 0.000000e+00 8.099160e+00
Na -8.099160e+00 4.049580e+00 -4.049580e+00
Na -6.074370e+00 6.074370e+00 -4.049580e+00
Na -4.049580e+00 8.099160e+00 -4.049580e+00
Na -8.099160e+00 2.024790e+00 -2.024790e+00
Na -6.074370e+00 4.049580e+00 -2.024790e+00
Na -4.049580e+00 6.074370e+00 -2.024790e+00
Na -2.024790e+00 8.099160e+00 -2.024790e+00
Na -8.099160e+00 0.000000e+00 0.000000e+00
Na -6.074370e+00 2.024790e+00 0.000000e+00
Na -4.049580e+00 4.049580e+00 0.000000e+00
Na -2.024790e+00 6.074370e+00 0.000000e+00
Na 0.000000e+00 8.099160e+00 0.000000e+00
Na -8.099160e+00 -2.024790e+00 2.024790e+00
Na -6.074370e+00 0.000000e+00 2.024790e+00
Na -4.049580e+00 2.024790e+00 2.024790e+00
Na -2.024790e+00 4.049580e+00 2.024790e+00
Na 0.000000e+00 6.074370e+00 2.024790e+00
Na 2.024790e+00 8.099160e+00 2.024790e+00
Na -8.099160e+00 -4.049580e+00 4.049580e+00
Na -6.074370e+00 -2.024790e+00 4.049580e+00
Na -4.049580e+00 0.000000e+00 4.049580e+00
Na -2.024790e+00 2.024790e+00 4.049580e+00
Na 0.000000e+00 4.049580e+00 4.049580e+00
Na 2.024790e+00 6.074370e+00 4.049580e+00
Na 4.049580e+00 8.099160e+00 4.049580e+00
Na -6.074370e+00 -4.049580e+00 6.074370e+00
Na -4.049580e+00 -2.024790e+00 6.074370e+00
Na -2.024790e+00 0.000000e+00 6.074370e+00
Na 0.000000e+00 2.024790e+00 6.074370e+00
Na 2.024790e+00 4.049580e+00 6.074370e+00

Na 4.049580e+00 6.074370e+00 6.074370e+00
Na -4.049580e+00 -4.049580e+00 8.099160e+00
Na -2.024790e+00 -2.024790e+00 8.099160e+00
Na 0.000000e+00 0.000000e+00 8.099160e+00
Na 2.024790e+00 2.024790e+00 8.099160e+00
Na 4.049580e+00 4.049580e+00 8.099160e+00
Na -8.099160e+00 4.049580e+00 0.000000e+00
Na -6.074370e+00 6.074370e+00 0.000000e+00
Na -4.049580e+00 8.099160e+00 0.000000e+00
Na -8.099160e+00 2.024790e+00 2.024790e+00
Na -6.074370e+00 4.049580e+00 2.024790e+00
Na -4.049580e+00 6.074370e+00 2.024790e+00
Na -2.024790e+00 8.099160e+00 2.024790e+00
Na -8.099160e+00 0.000000e+00 4.049580e+00
Na -6.074370e+00 2.024790e+00 4.049580e+00
Na -4.049580e+00 4.049580e+00 4.049580e+00
Na -2.024790e+00 6.074370e+00 4.049580e+00
Na 0.000000e+00 8.099160e+00 4.049580e+00
Na -6.074370e+00 0.000000e+00 6.074370e+00
Na -4.049580e+00 2.024790e+00 6.074370e+00
Na -2.024790e+00 4.049580e+00 6.074370e+00
Na 0.000000e+00 6.074370e+00 6.074370e+00
Na -4.049580e+00 0.000000e+00 8.099160e+00
Na -2.024790e+00 2.024790e+00 8.099160e+00
Na 0.000000e+00 4.049580e+00 8.099160e+00
Na -8.099160e+00 4.049580e+00 4.049580e+00
Na -6.074370e+00 6.074370e+00 4.049580e+00
Na -4.049580e+00 8.099160e+00 4.049580e+00
Na -6.074370e+00 4.049580e+00 6.074370e+00
Na -4.049580e+00 6.074370e+00 6.074370e+00
Na -4.049580e+00 4.049580e+00 8.099160e+00

Atomic coordinates of Na 0.75 nm nanoparticle

Na 2.024790e+00 -4.049580e+00 -6.074370e+00
Na 4.049580e+00 -2.024790e+00 -6.074370e+00
Na 2.024790e+00 -6.074370e+00 -4.049580e+00
Na 4.049580e+00 -4.049580e+00 -4.049580e+00
Na 6.074370e+00 -2.024790e+00 -4.049580e+00
Na 4.049580e+00 -6.074370e+00 -2.024790e+00
Na 6.074370e+00 -4.049580e+00 -2.024790e+00
Na -2.024790e+00 -4.049580e+00 -6.074370e+00
Na 0.000000e+00 -2.024790e+00 -6.074370e+00
Na 2.024790e+00 0.000000e+00 -6.074370e+00
Na 4.049580e+00 2.024790e+00 -6.074370e+00
Na -2.024790e+00 -6.074370e+00 -4.049580e+00
Na 0.000000e+00 -4.049580e+00 -4.049580e+00
Na 2.024790e+00 -2.024790e+00 -4.049580e+00
Na 4.049580e+00 0.000000e+00 -4.049580e+00
Na 6.074370e+00 2.024790e+00 -4.049580e+00
Na 0.000000e+00 -6.074370e+00 -2.024790e+00
Na 2.024790e+00 -4.049580e+00 -2.024790e+00
Na 4.049580e+00 -2.024790e+00 -2.024790e+00
Na 6.074370e+00 0.000000e+00 -2.024790e+00
Na 2.024790e+00 -6.074370e+00 0.000000e+00
Na 4.049580e+00 -4.049580e+00 0.000000e+00
Na 6.074370e+00 -2.024790e+00 0.000000e+00
Na 4.049580e+00 -6.074370e+00 2.024790e+00
Na 6.074370e+00 -4.049580e+00 2.024790e+00
Na -4.049580e+00 -2.024790e+00 -6.074370e+00
Na -2.024790e+00 0.000000e+00 -6.074370e+00
Na 0.000000e+00 2.024790e+00 -6.074370e+00
Na 2.024790e+00 4.049580e+00 -6.074370e+00
Na -4.049580e+00 -4.049580e+00 -4.049580e+00

Na -2.024790e+00 -2.024790e+00 -4.049580e+00
Na 0.000000e+00 0.000000e+00 -4.049580e+00
Na 2.024790e+00 2.024790e+00 -4.049580e+00
Na 4.049580e+00 4.049580e+00 -4.049580e+00
Na -4.049580e+00 -6.074370e+00 -2.024790e+00
Na -2.024790e+00 -4.049580e+00 -2.024790e+00
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Atomic coordinates of Na 0.50 nm nanoparticle

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