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Online supporting information for:

First principles molecular dynamics simulations of UCl_n–$MgCl_2$ (n=3, 4) molten salts

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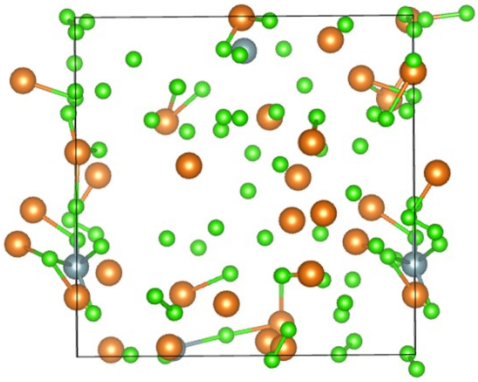
Initial structures from Packmol and final snapshots from FPMD.
Color code: U, gray; Mg, brown, Cl, green.

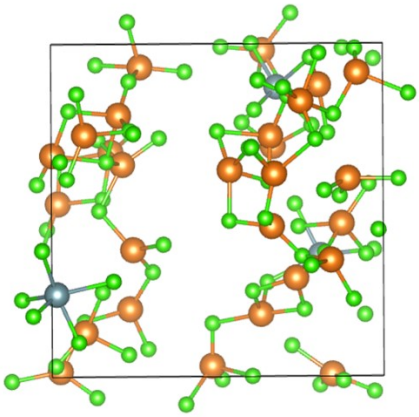
UCl_3–$MgCl_2$, x(UCl_3) = 0.1 2
UCl_3–$MgCl_2$, x(UCl_3) = 0.2 2
UCl_3–$MgCl_2$, x(UCl_3) = 0.3 3
UCl_3–$MgCl_2$, x(UCl_3) = 0.4 3
UCl_3–$MgCl_2$, x(UCl_3) = 0.5 4
UCl_3–$MgCl_2$, x(UCl_3) = 0.75 4
UCl_3–$MgCl_2$, x(UCl_3) = 1.0 5
UCl_4–$MgCl_2$, x(UCl_4) = 0.1 5
UCl_4–$MgCl_2$, x(UCl_4) = 0.2 6
UCl_4–$MgCl_2$, x(UCl_4) = 0.3 6
UCl_4–$MgCl_2$, x(UCl_4) = 0.4 7
UCl_4–$MgCl_2$, x(UCl_4) = 0.5 7
UCl_4–$MgCl_2$, x(UCl_4) = 0.75 8
UCl_4–$MgCl_2$, x(UCl_4) = 1.0 8

UCl_3–$MgCl_2$, x(UCl_3) = 0.1

Initial structure

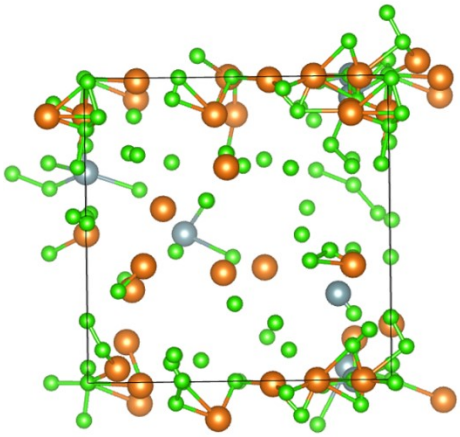


Final snapshot



UCl_3–$MgCl_2$, x(UCl_3) = 0.2

Initial structure



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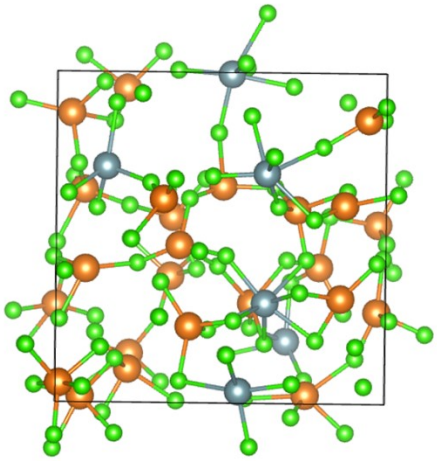
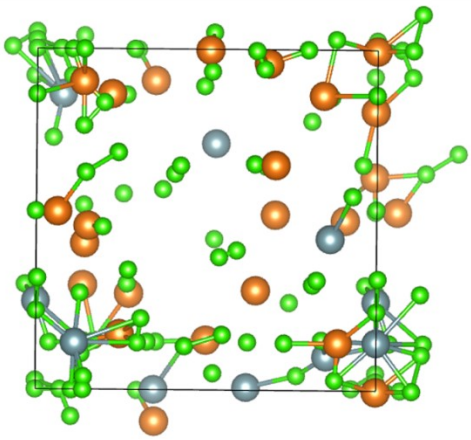


UCl_3–$MgCl_2$, x(UCl_3) = 0.3

Initial structure



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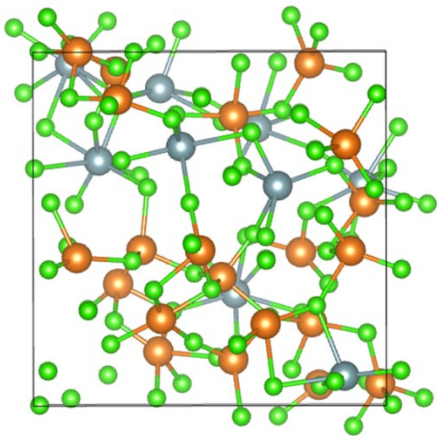
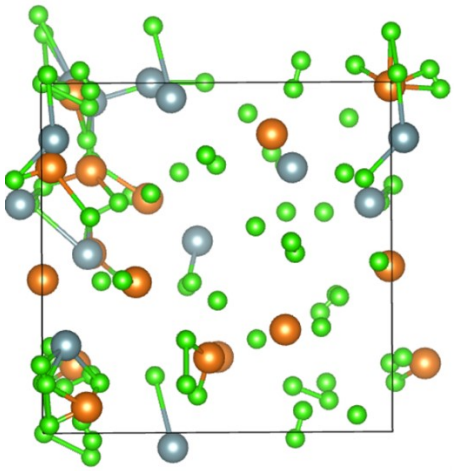


UCl_3–$MgCl_2$, x(UCl_3) = 0.4

Initial structure



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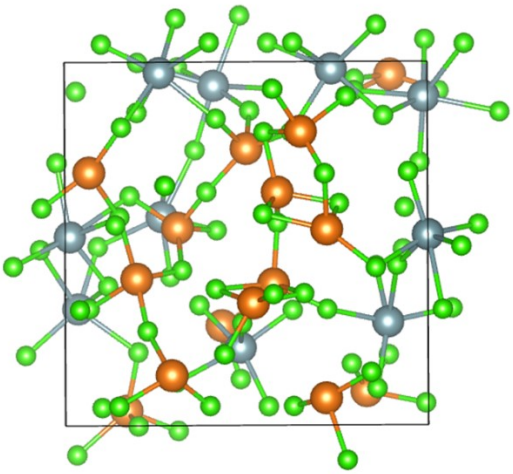
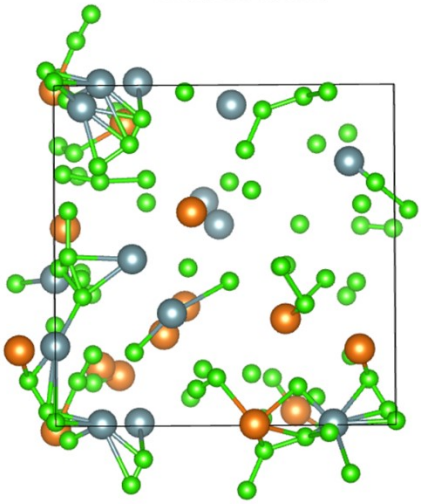


UCl_3–$MgCl_2$, x(UCl_3) = 0.5

Initial structure



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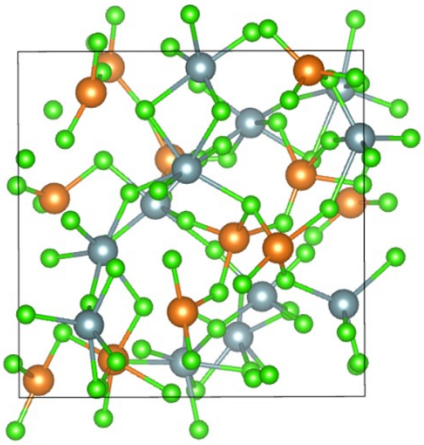
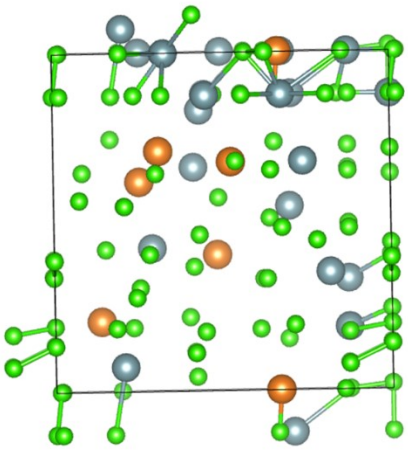


UCl_3–$MgCl_2$, x(UCl_3) = 0.75

Initial structure



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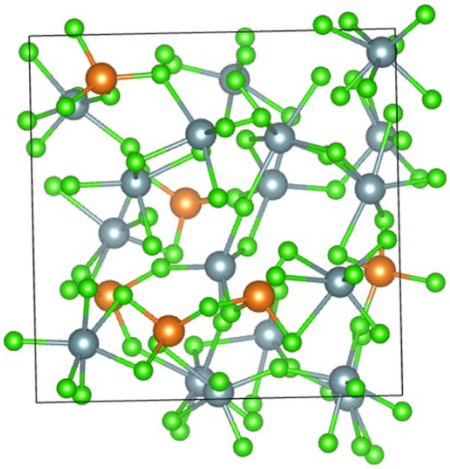
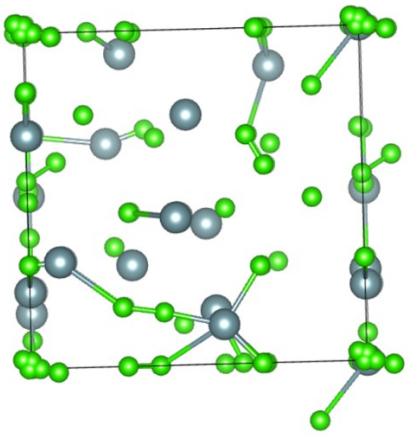


UCl_3–$MgCl_2$, x(UCl_3) = 1.0

Initial structure



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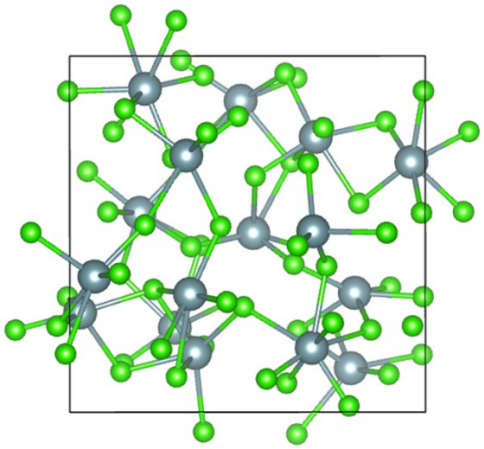
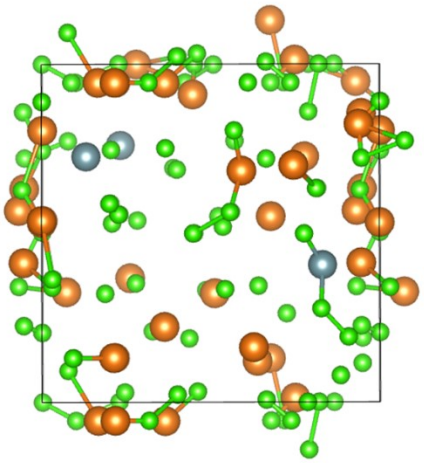


UCl_4–$MgCl_2$, x(UCl_4) = 0.1

Initial structure



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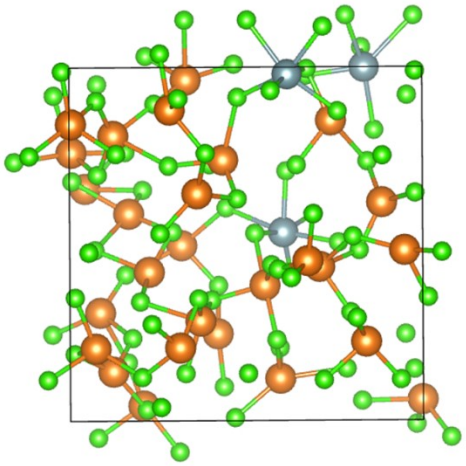
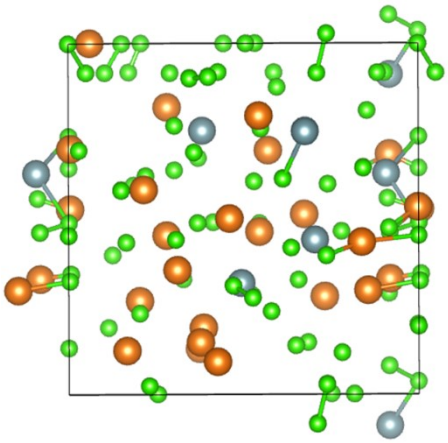


UCl_4–$MgCl_2$, x(UCl_4) = 0.2

Initial structure



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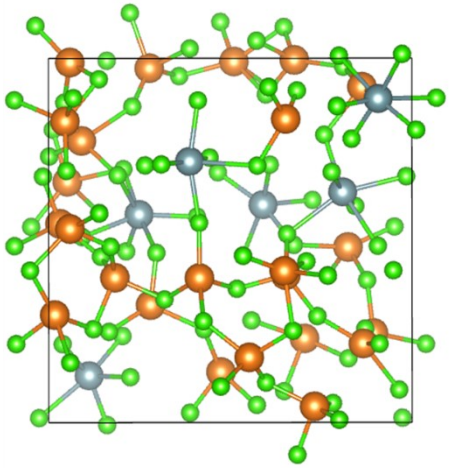
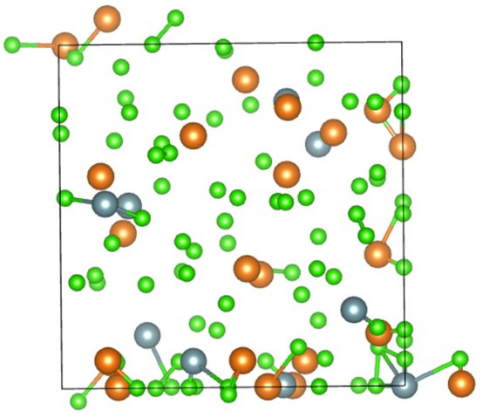


UCl_4–$MgCl_2$, x(UCl_4) = 0.3

Initial structure



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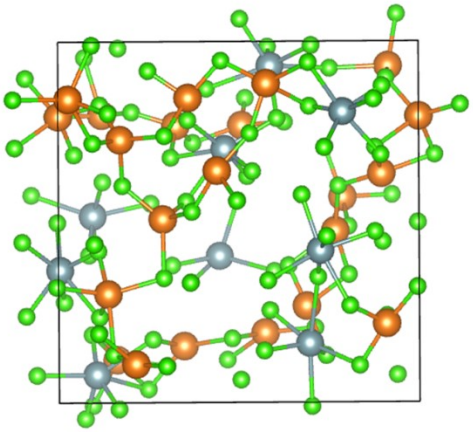
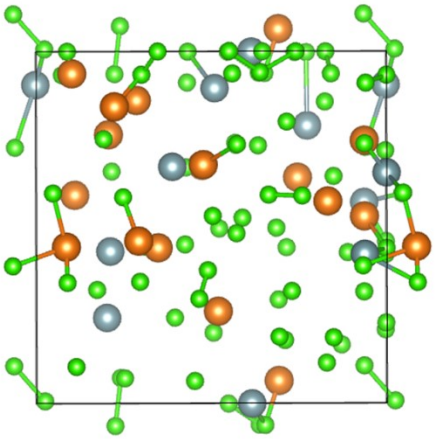


UCl_4–$MgCl_2$, x(UCl_4) = 0.4

Initial structure



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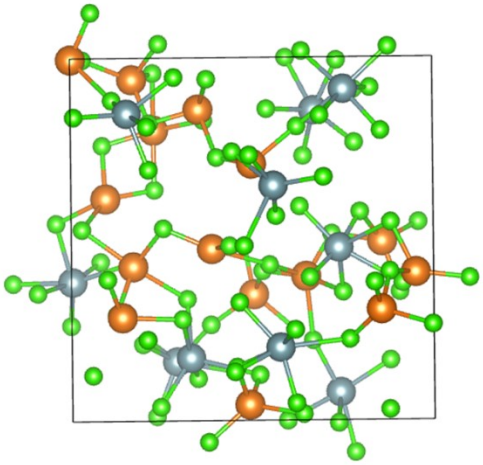
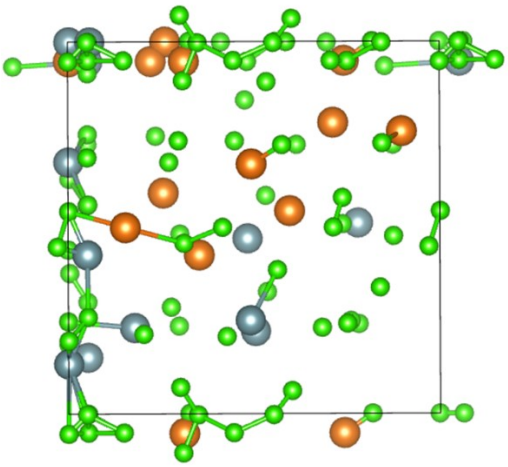


UCl_4–$MgCl_2$, x(UCl_4) = 0.5

Initial structure



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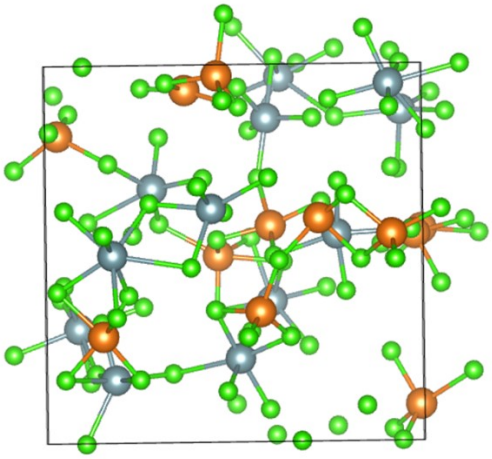
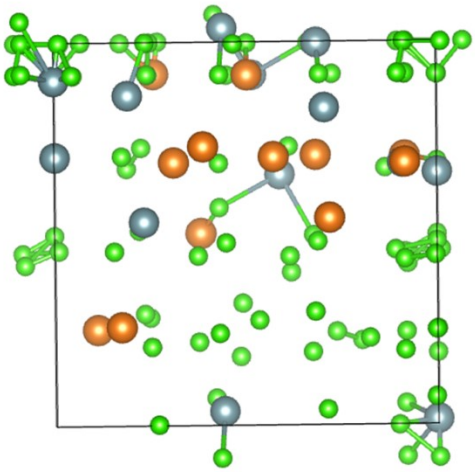
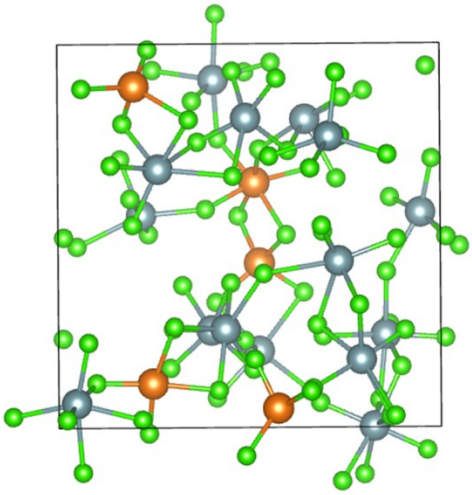


UCl_4–$MgCl_2$, x(UCl_4) = 0.75

Initial structure

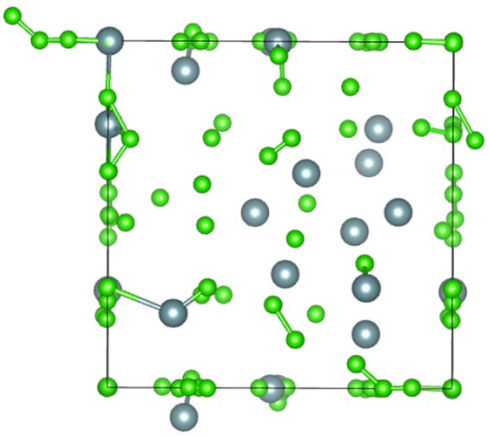
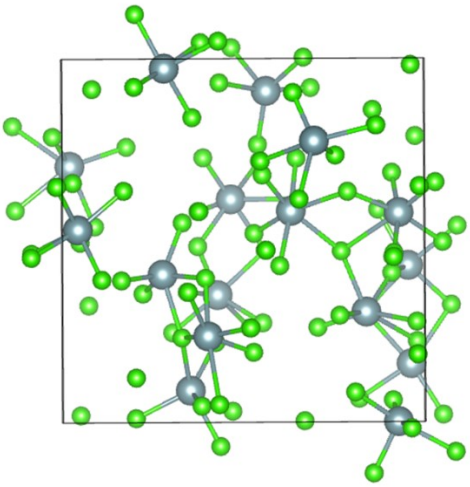


Final snapshot



UCl_4–$MgCl_2$, x(UCl_4) = 1.0

Initial structure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