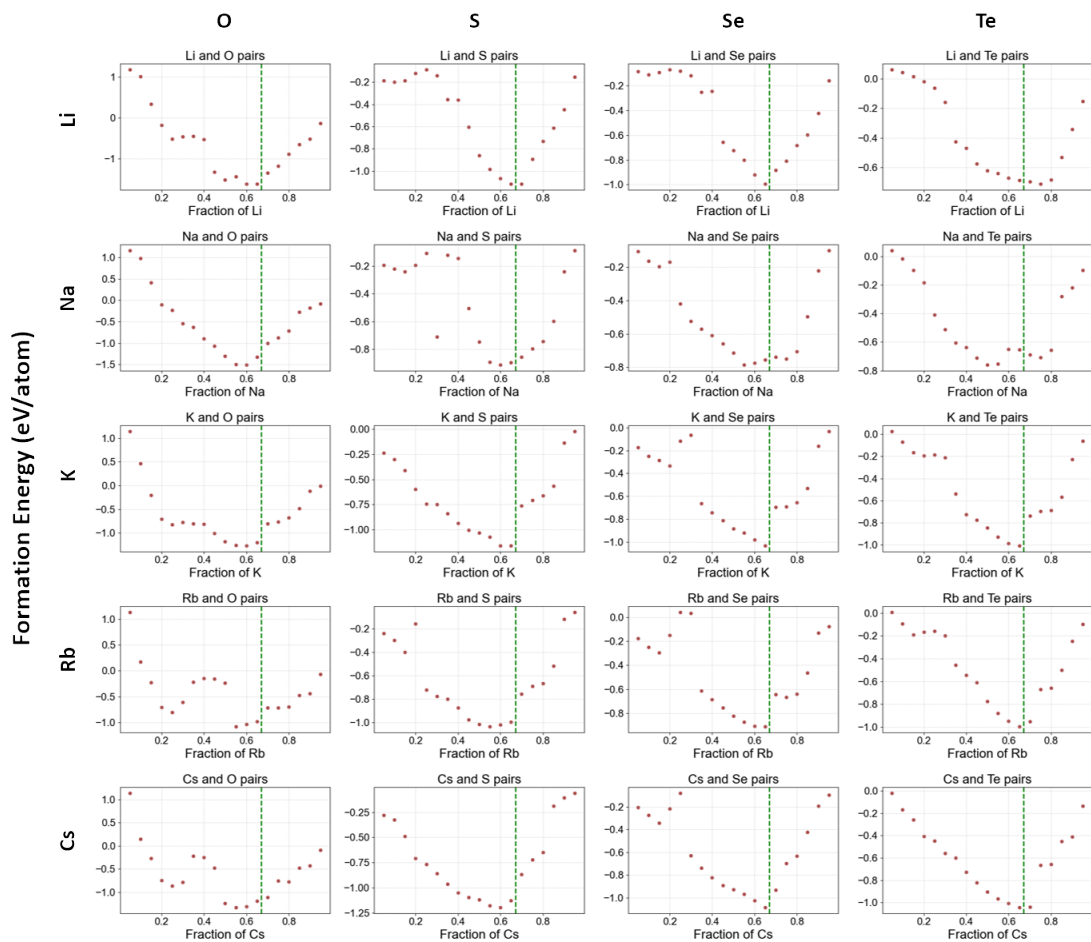


Supplementary Information: XElemNet: Towards Explainable AI for Deep Neural Networks in Materials Science

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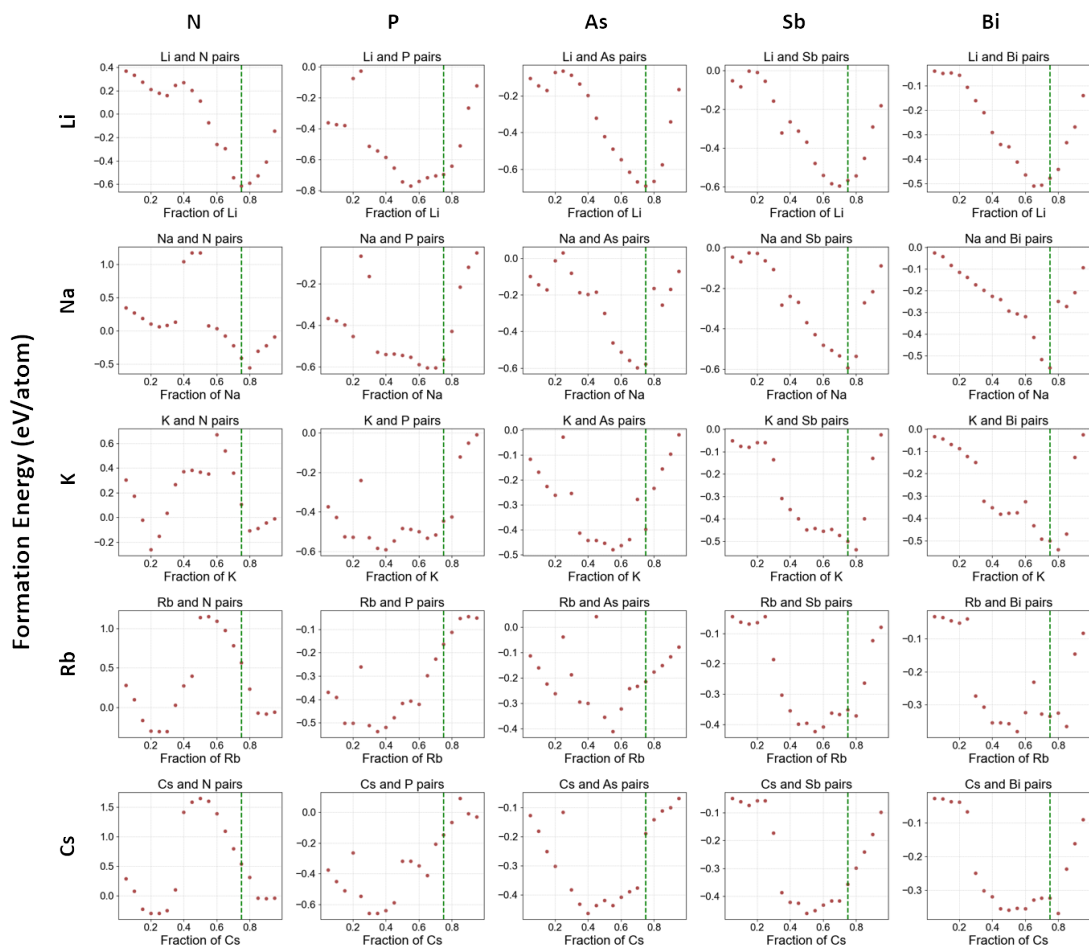
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Supplementary Figure 1: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 1 and element "B" from group 6.

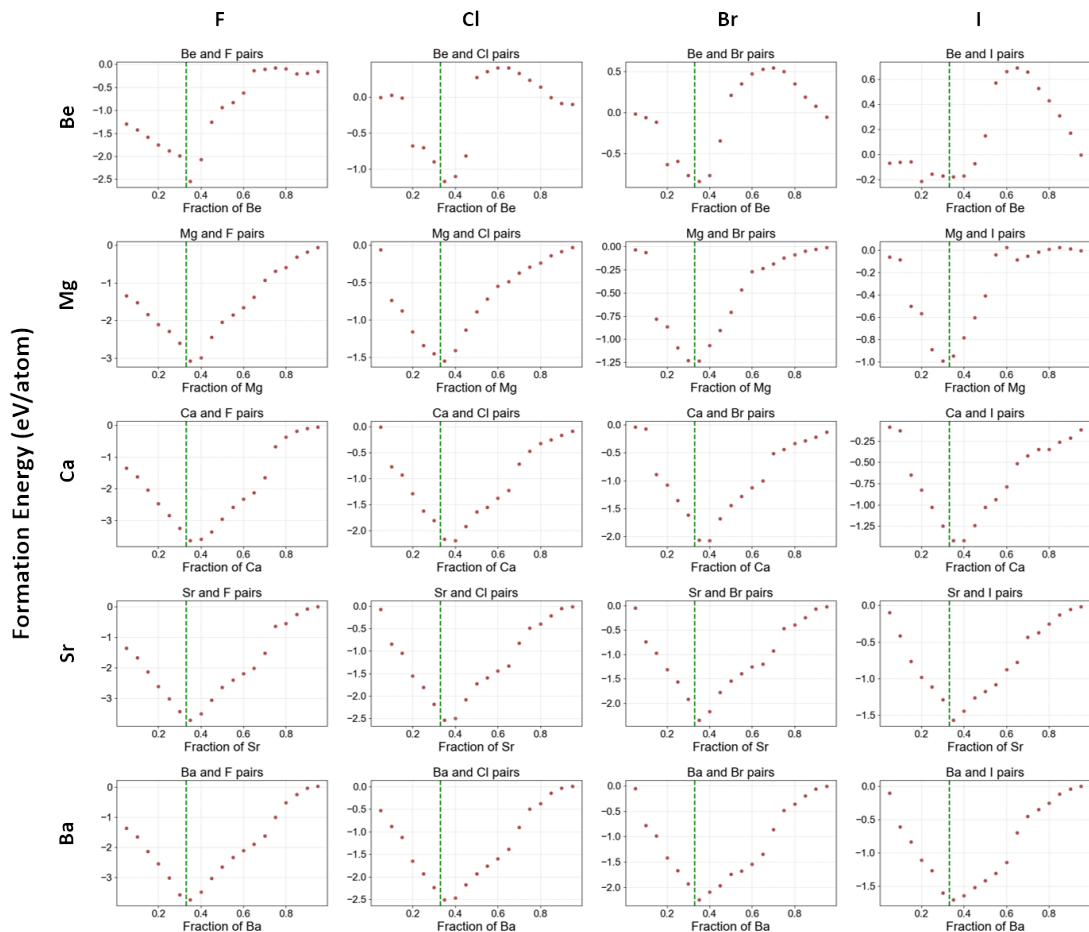
Green lines at $x_e = 0.67$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 2: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 1 and element "B" from group 5.

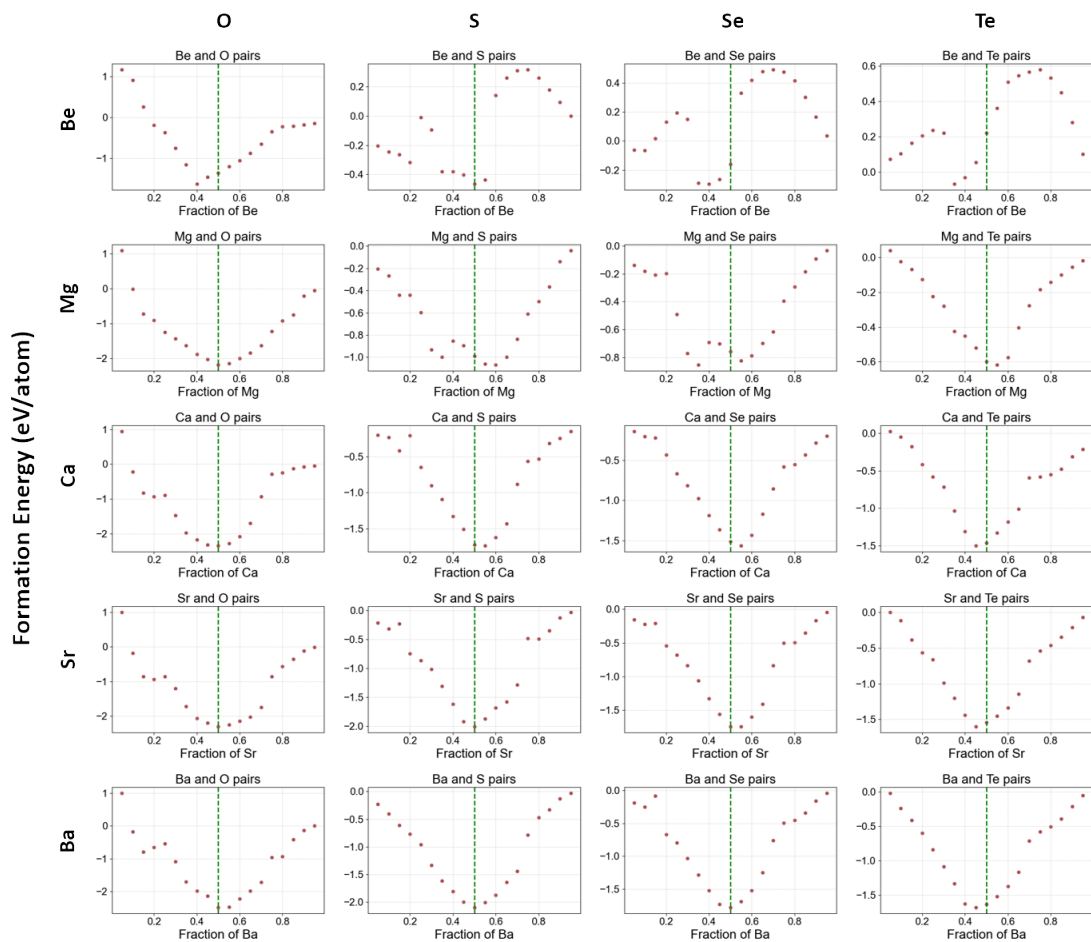
Green lines at $x_e = 0.75$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 3: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 2 and element "B" from group 7.

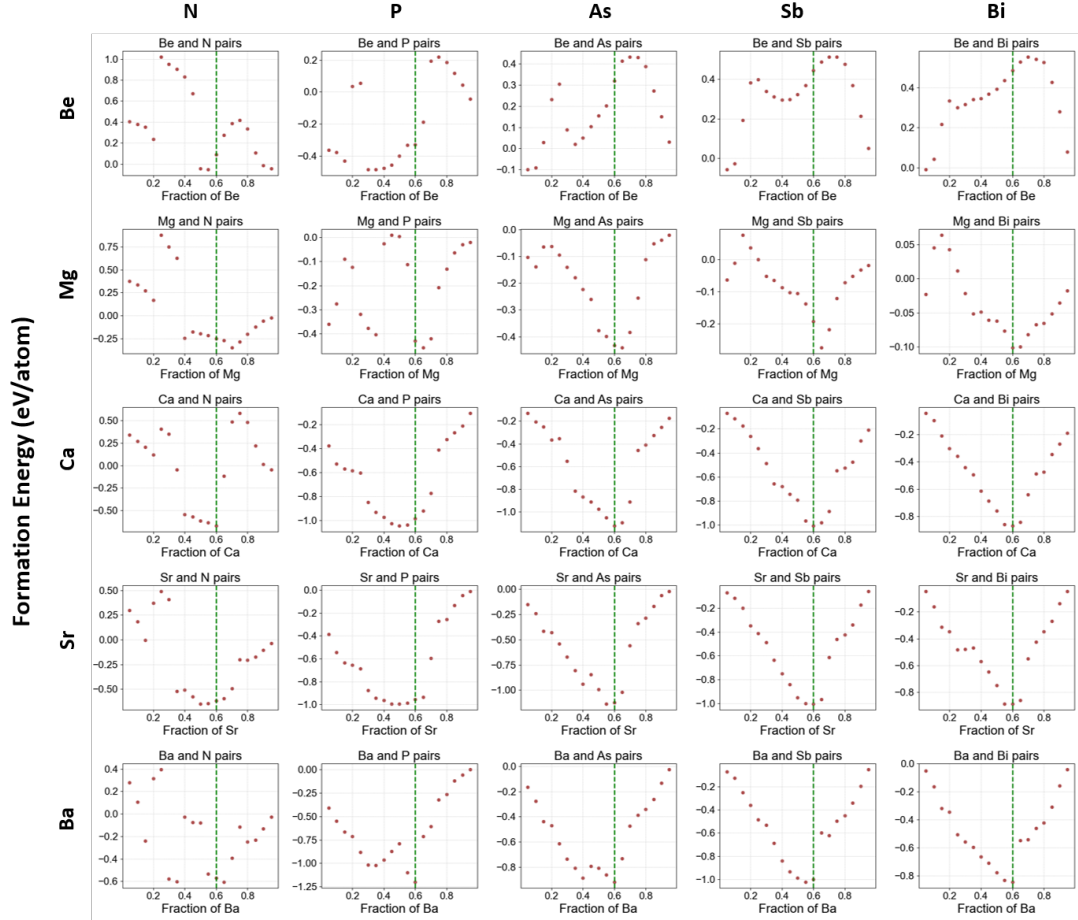
Green lines at $x_e = 0.33$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 4: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 2 and element "B" from group 6.

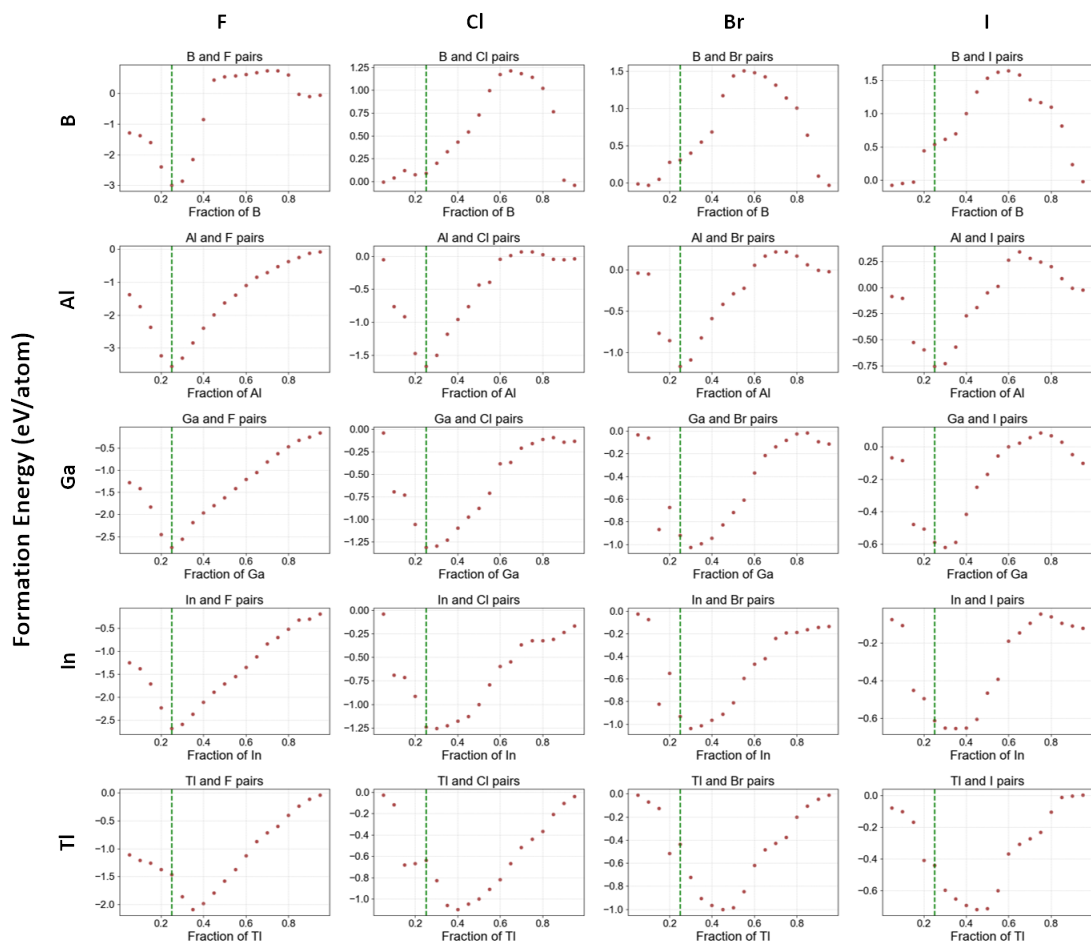
Green lines at $x_e = 0.50$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 5: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 2 and element "B" from group 5.

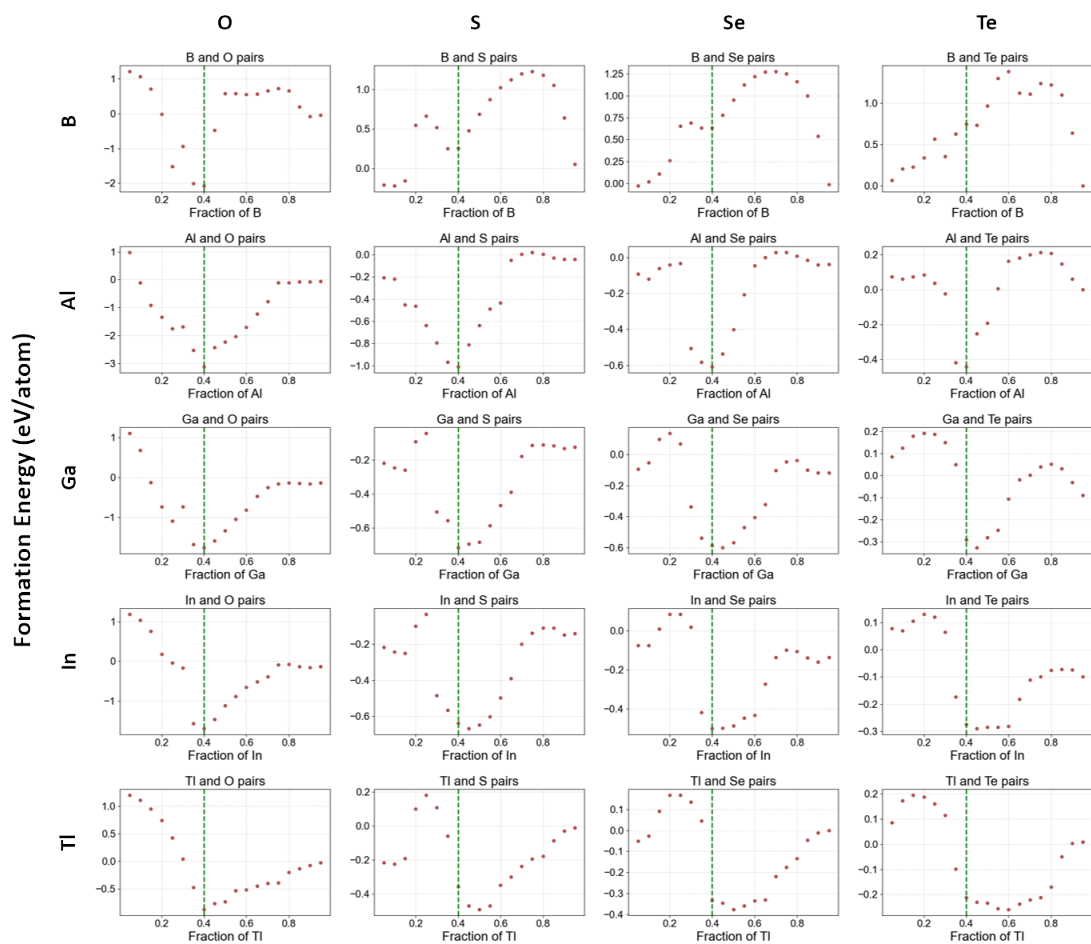
Green lines at $x_e = 0.60$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 6: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 3 and element "B" from group 7.

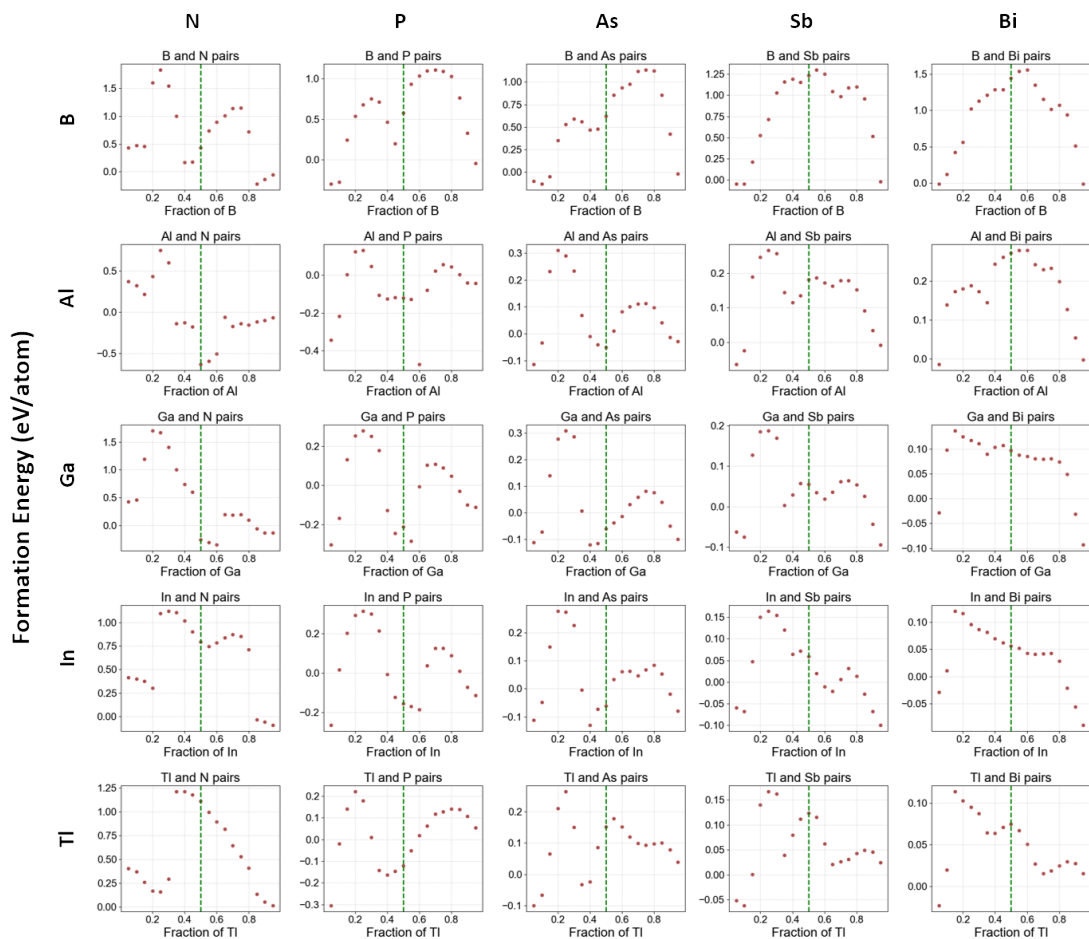
Green lines at $x_e = 0.25$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 7: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 3 and element "B" from group 6.

Green lines at $x_e = 0.40$ indicate the elemental fraction expected to have the lowest formation energy.



Supplementary Figure 8: Predicted convex hulls for the secondary binary dataset (A_xB_y).

Red dots denote pairs with element "A" from group 3 and element "B" from group 5.

Green lines at $x_e = 0.50$ indicate the elemental fraction expected to have the lowest formation energy.