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Interpretable Attention-based Transfer Learning in Plasma Catalysis: A Study on the Role of Surface Charge†

Supporting Information (SI)

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† Supplementary Information available: [details of any supplementary information available should be included here]. See DOI: 00.0000/00000000.

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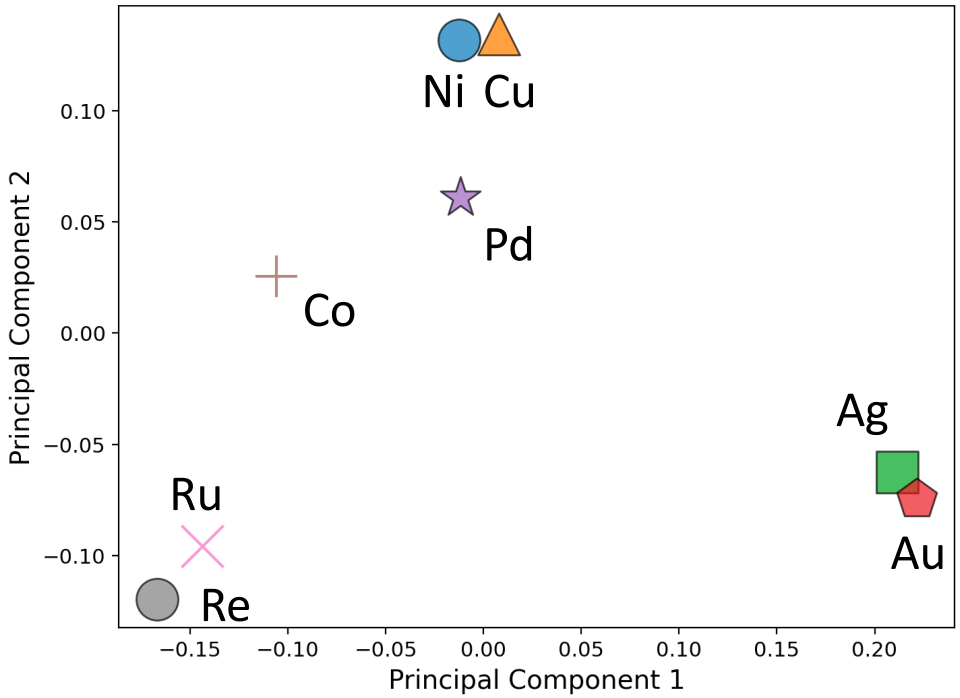

Fig. SP1 The 2-dimensional contour, based on principal components 1 and 2, represents the projection of the attention scores onto a 3-dimensional space.

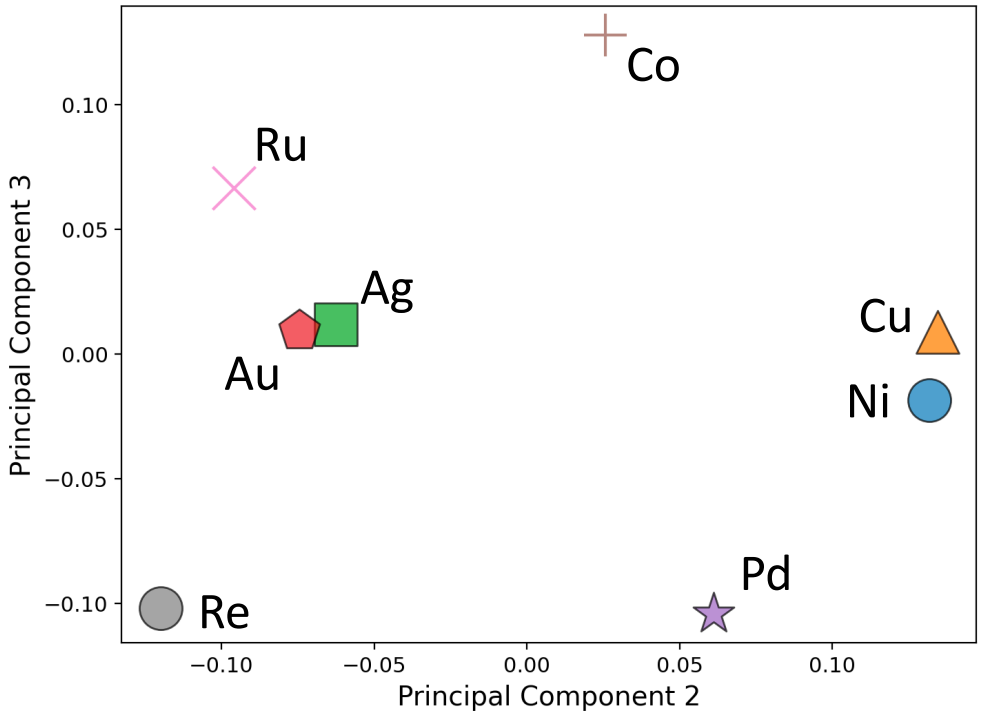

Fig. SP2 The 2-dimensional contour, based on principal components 2 and 3, represents the projection of the attention scores onto a 3-dimensional space.

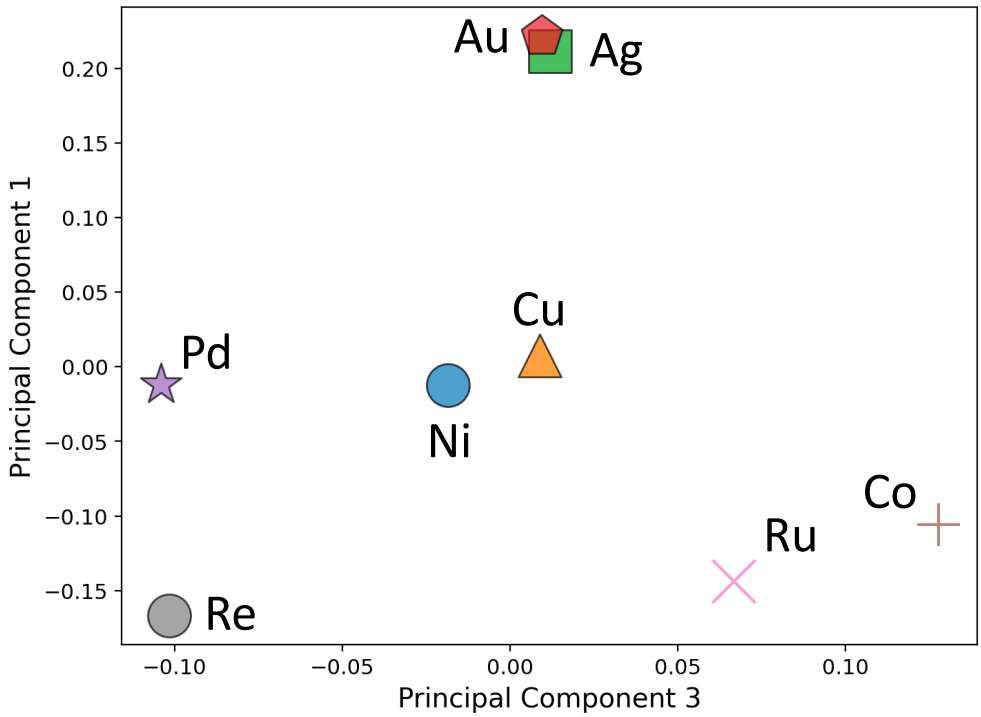

Fig. SP3 The 2-dimensional contour, based on principal components 1 and 3, represents the projection of the attention scores onto a 3-dimensional space.

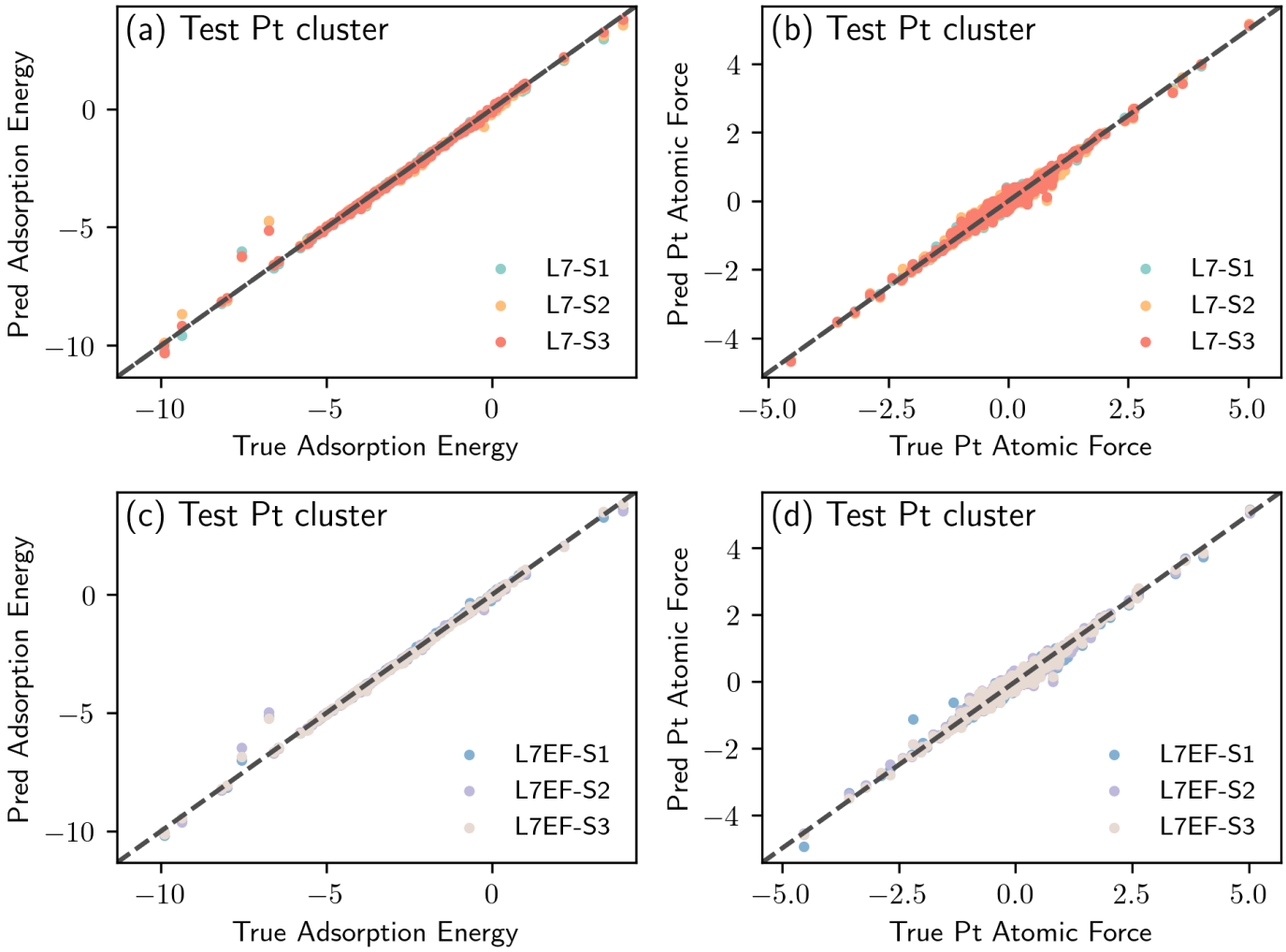

Fig. SP4 Parity plots of the adsorption energy and atomic force predictions for the test Pt metal clusters. (a) Actual adsorption energy against its corresponding predicted values for model L7 fine-tuned using the transfer learning strategies S1, S2 and S3. (b) Actual atomic force against its corresponding predicted values for model L7 fine-tuned using the transfer learning strategies S1, S2 and S3. (c) Actual adsorption energy against its corresponding predicted values for model L7EF fine-tuned using the transfer learning strategies S1, S2 and S3. (d) Actual atomic force against its corresponding predicted values for model L7EF fine-tuned using the transfer learning strategies S1, S2 and S3.