Machine-Learning-Guided Prediction of CO Adsorption Energetics for the Rational Design of Methanol Oxidation Catalysts

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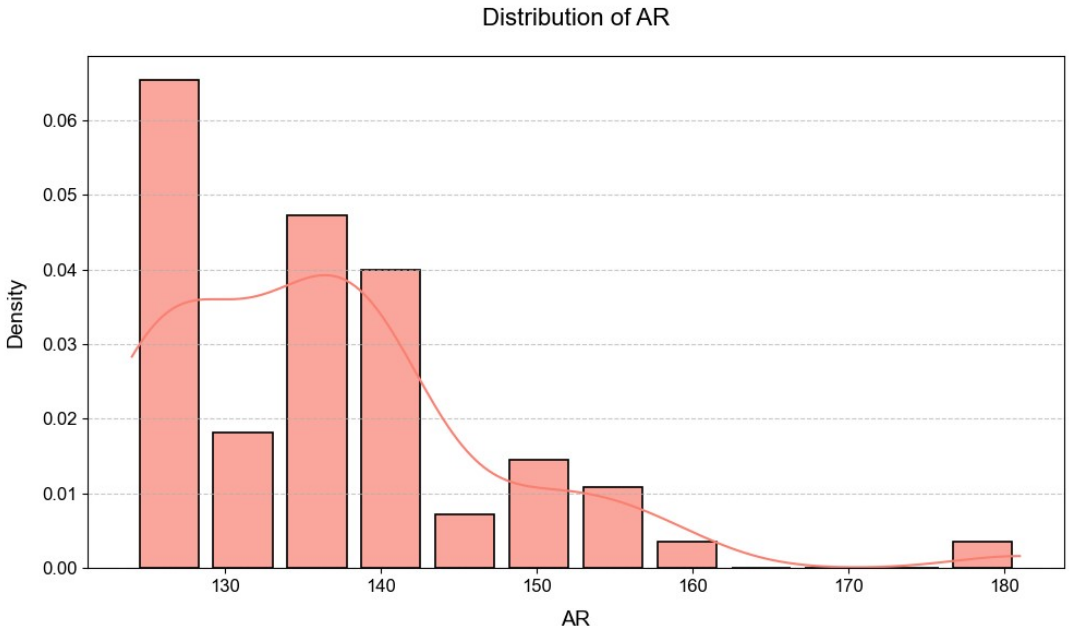

S1. Histogram and KDE depicting the statistical distribution of atomic radius. A dominant peak appears around 125, corresponding to the primary concentration region, while the tail gradually disperses toward larger values, suggesting moderate variability in geometric descriptors.

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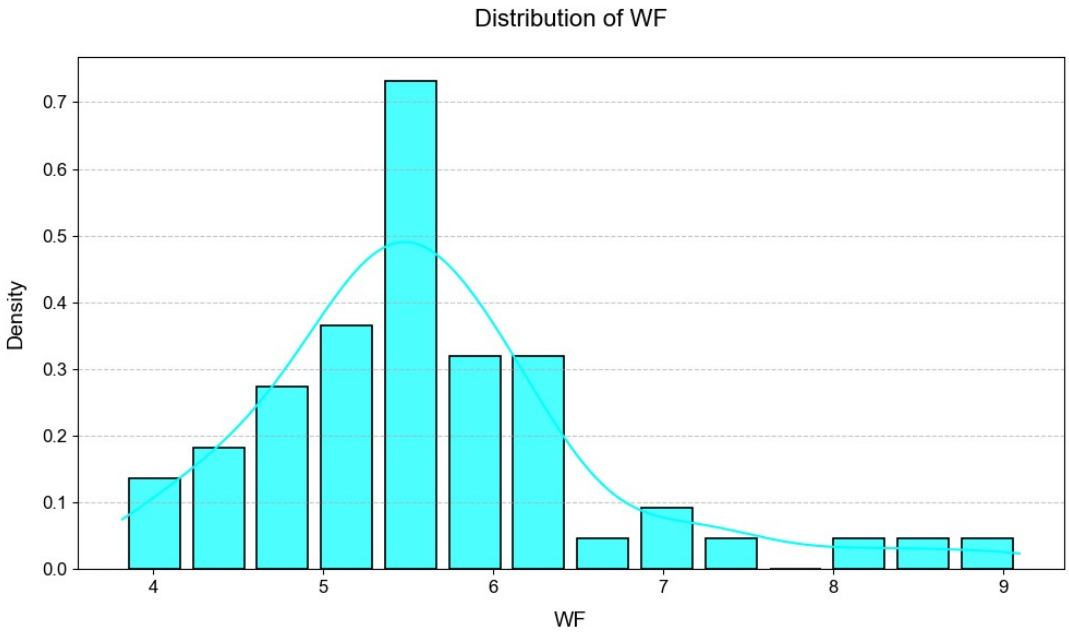
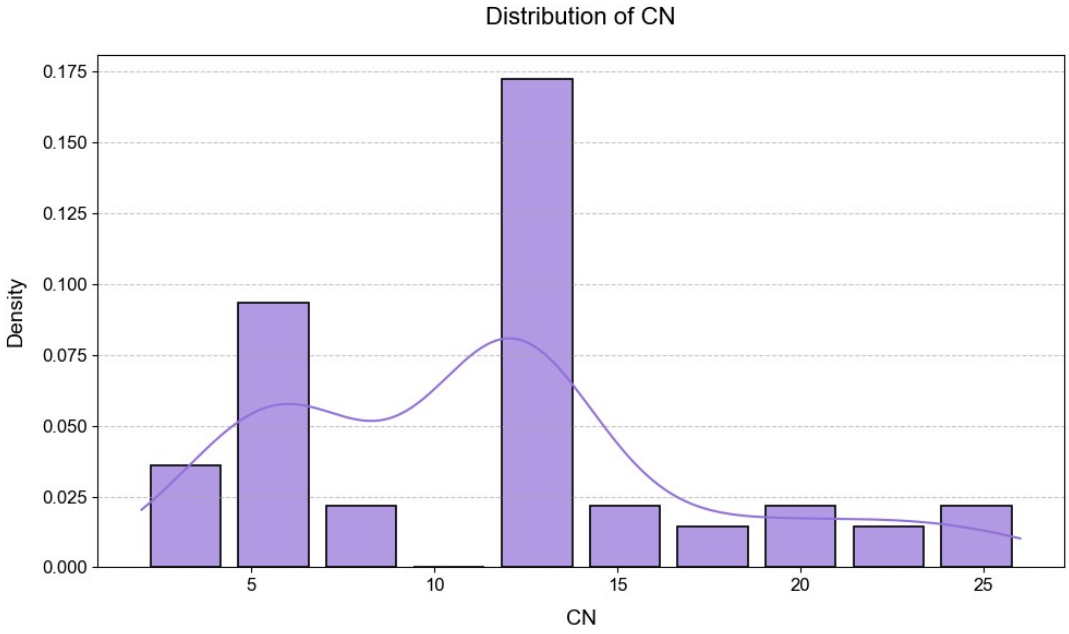
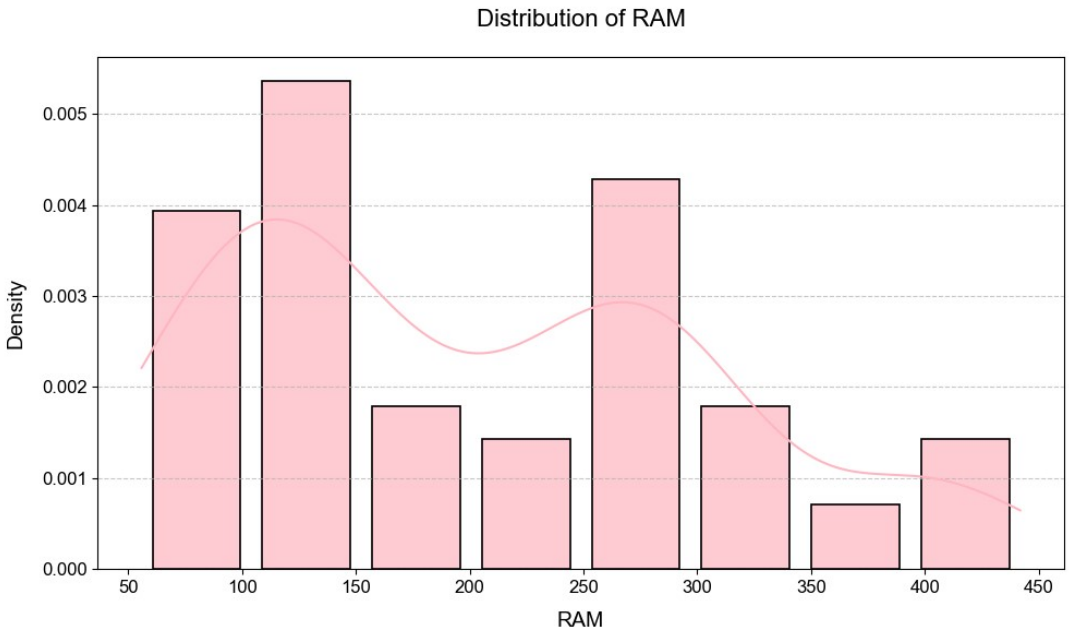


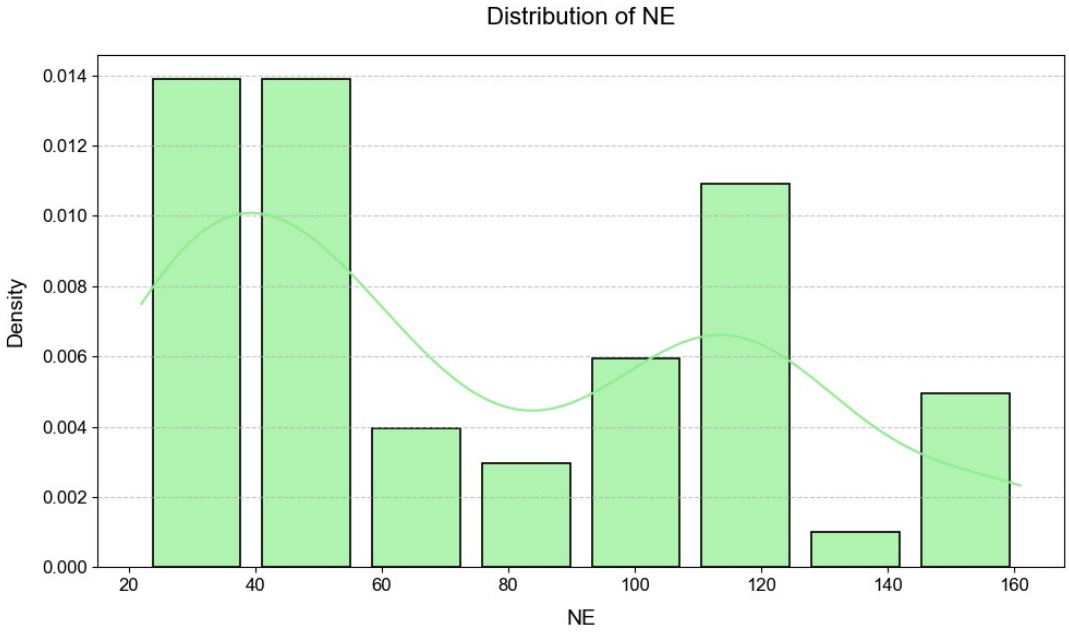
S2. Histogram and KDE showing the statistical distribution of work function values. WF displays a pronounced density maximum around 5 eV, indicating a well-defined central region and moderate dispersion in surface electronic potential across different catalyst systems.



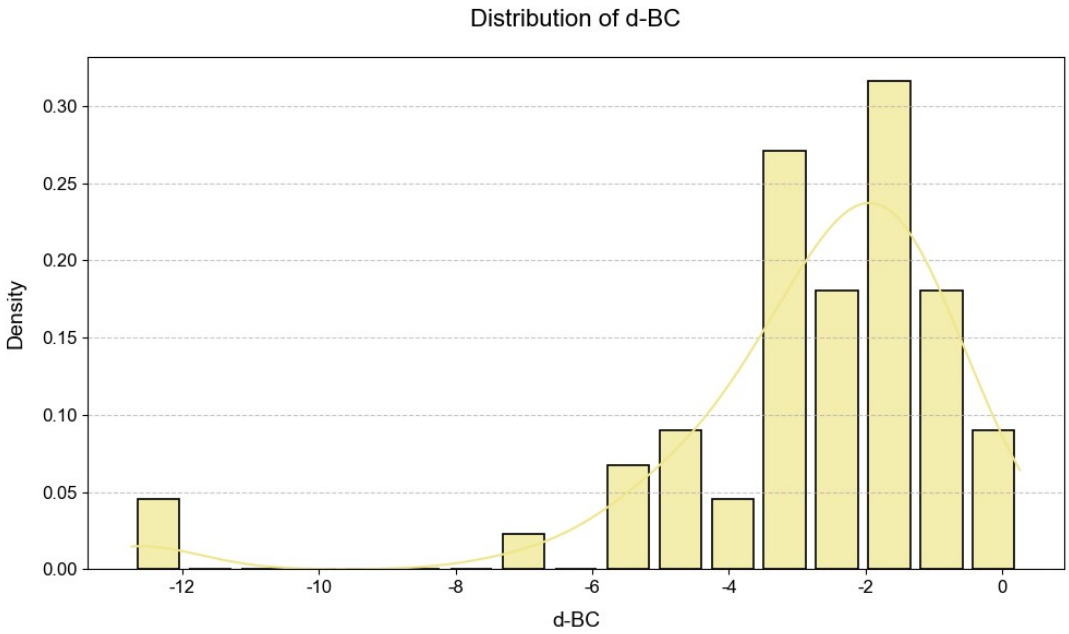
S3. Histogram and KDE presenting the distribution of coordination number. CN values are predominantly concentrated in the range of 10 – 15, forming a clear main peak with a gradually decaying tail, which captures the variation in local coordination environments of the catalyst surfaces.



S4. Histogram and KDE of relative atomic mass values. RAM shows a primary density maximum near 100, along with a secondary peak around 250, indicating a multimodal distribution that reflects the presence of both light and heavy metal elements in the dataset.



S5. Histogram and KDE illustrating the distribution of electron number across the dataset. The majority of NE values are concentrated in the range of 20 – 40, with an overall multimodal distribution, indicating distinct electronic characteristics among different catalyst compositions.



S6. Histogram and kernel density estimation (KDE) illustrating the statistical distribution of d-band center values in the dataset. The distribution exhibits a well-defined central region with a gradually decaying tail, reflecting variations in the electronic structure of the catalyst surfaces.