

Supplementary information

Neural network interpolation of exchange-correlation functional

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S1

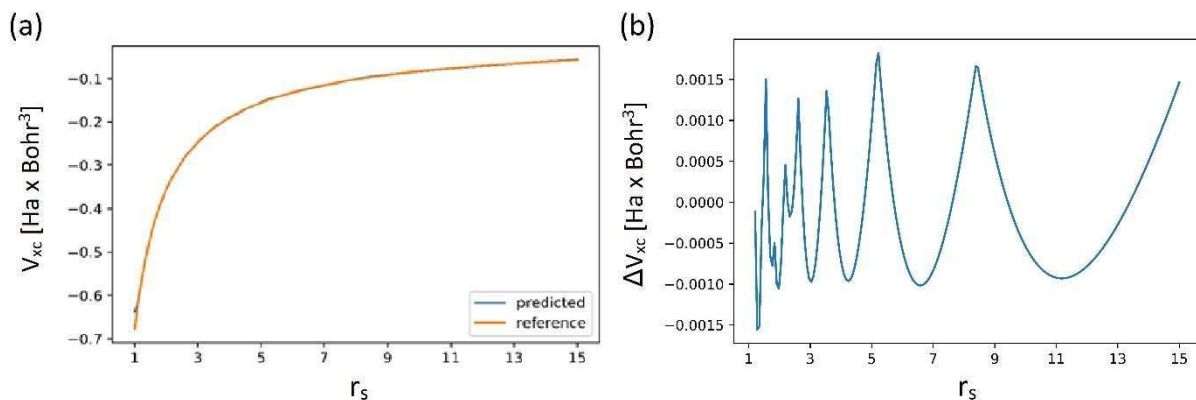


Figure S1. (a) LDA exchange-correlation potential versus r_s . Blue line – exchange-correlation potential obtained from NN, orange line – reference analytical LDA exchange-correlation potential. (b) Difference between exchange-correlation obtained from NN and reference analytical LDA exchange-correlation potential.

S2

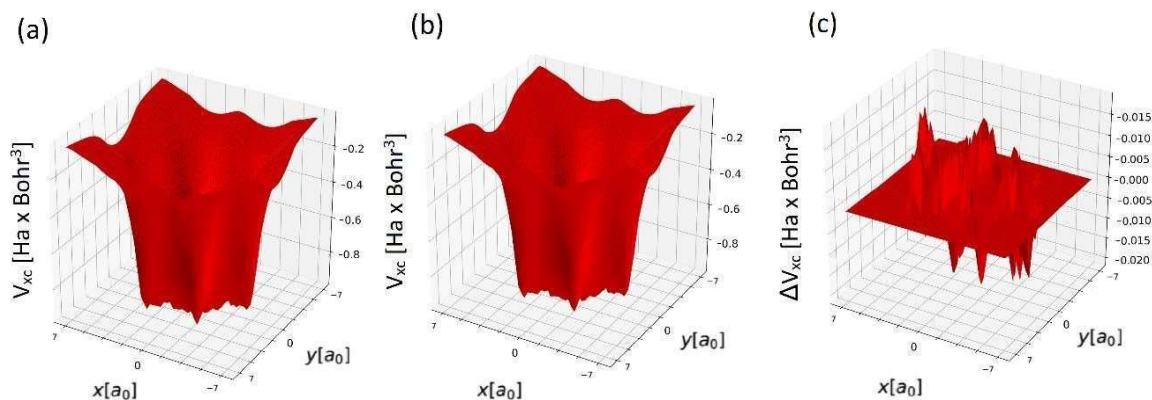


Figure S2. (a) Slice of LDA exchange-correlation initial potential for benzene at $z = 0$. (b) Slice at $z = 0$ of LDA exchange-correlation potential for 5x5x5 density cube rotated by 90 degrees along z axis passing through the centre of the cube. (c) Difference between slices specified in (a) and (b)