

Co₃O₄ (111) surfaces in contact with water: Molecular dynamics study of the surface chemistry and structure at room temperature

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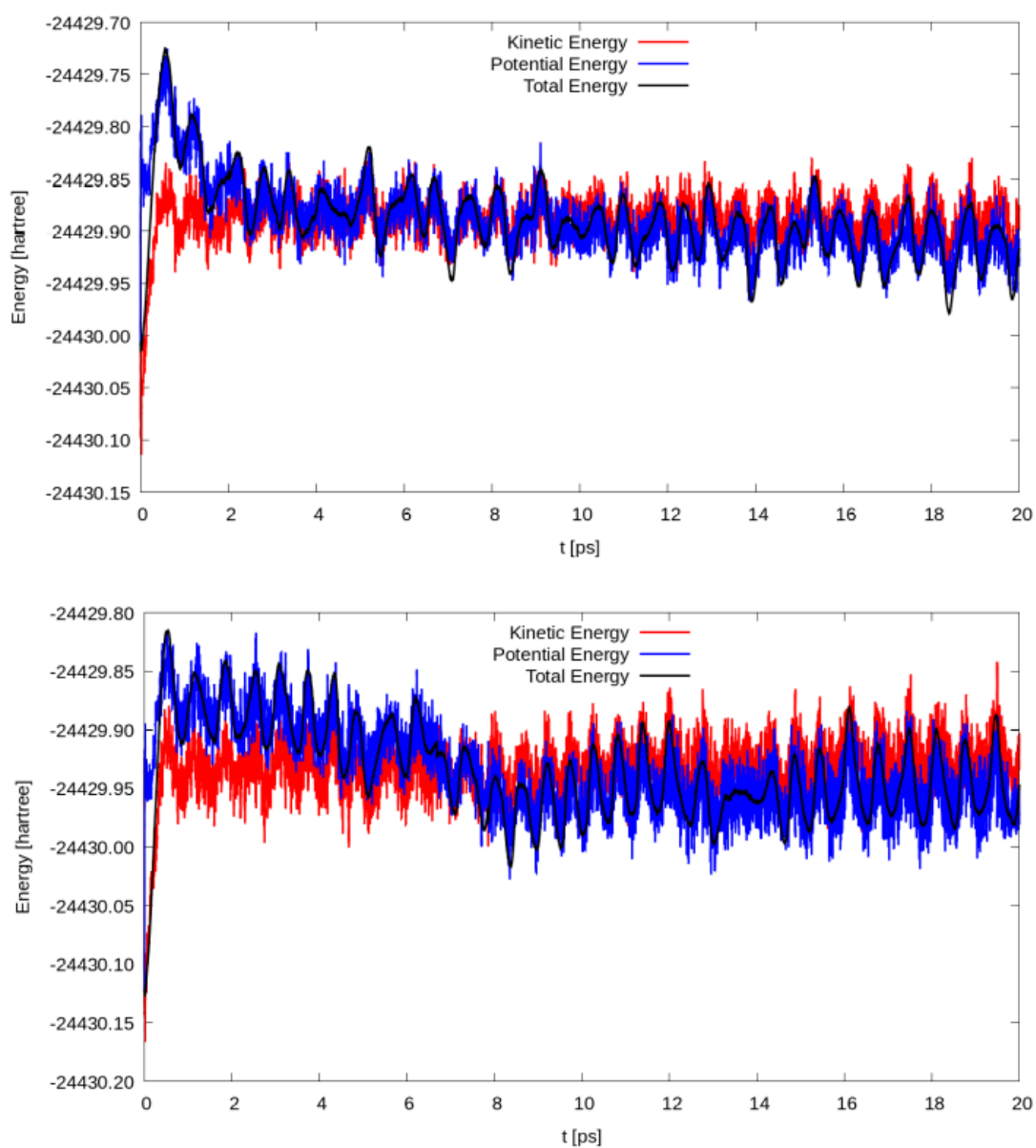


Figure S1: Kinetic, potential and total energies of the water covered A (top) and B- (bottom) terminations during the 20 ps simulations

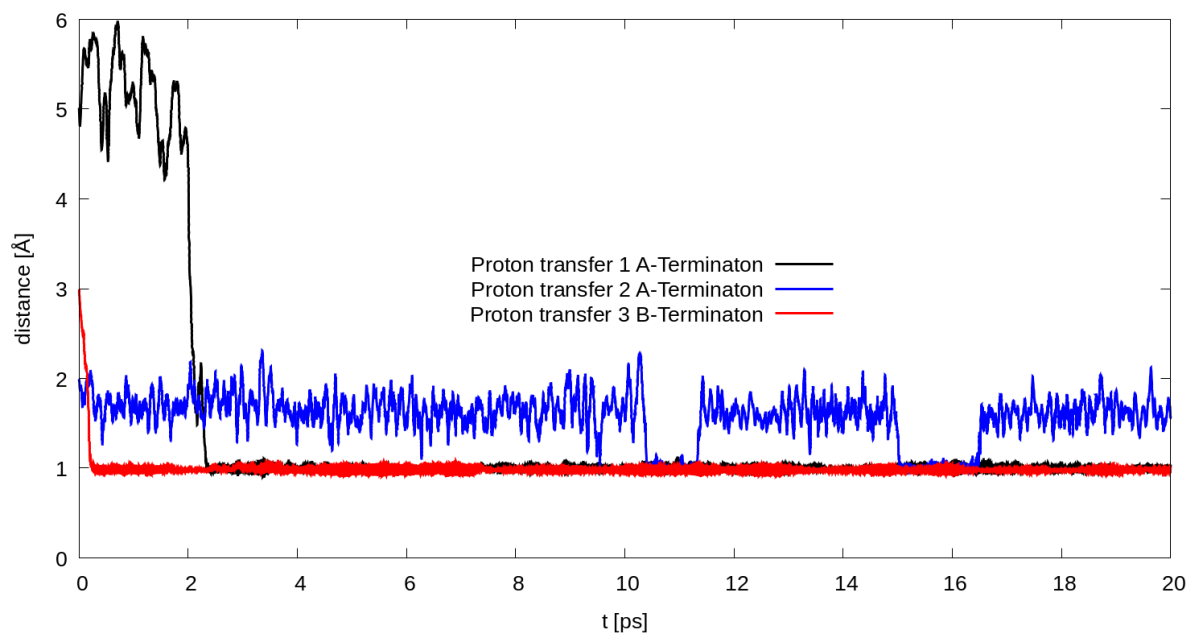


Figure S2: Time evolution of the surface oxygens to water Hydrogens (Os-H) bond distances from the simulations on the A- and B-terminated Co_3O_4 (111)/ H_2O interface. On the A termination, Proton transfer 1 denotes the transfer happening on the surface oxygens Os1, while Proton transfer 2 denotes the one happening on surface oxygens Os2

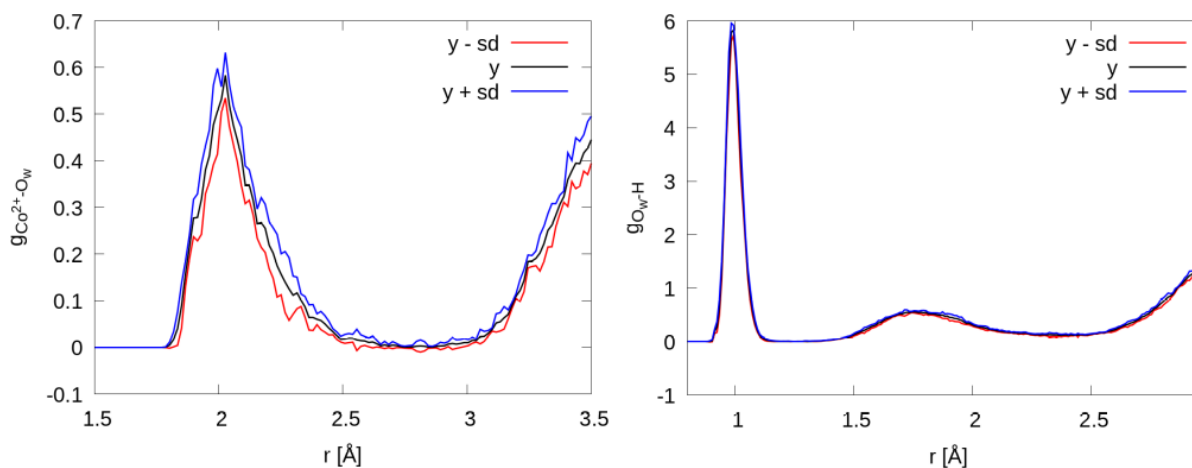


Figure S3: Average value of the radial distribution functions reported together with the standard deviation (sd), of the Co^{2+} to water oxygens O_w distances (left) and of the water oxygens to water hydrogens distances (right), on the A-terminated surface.

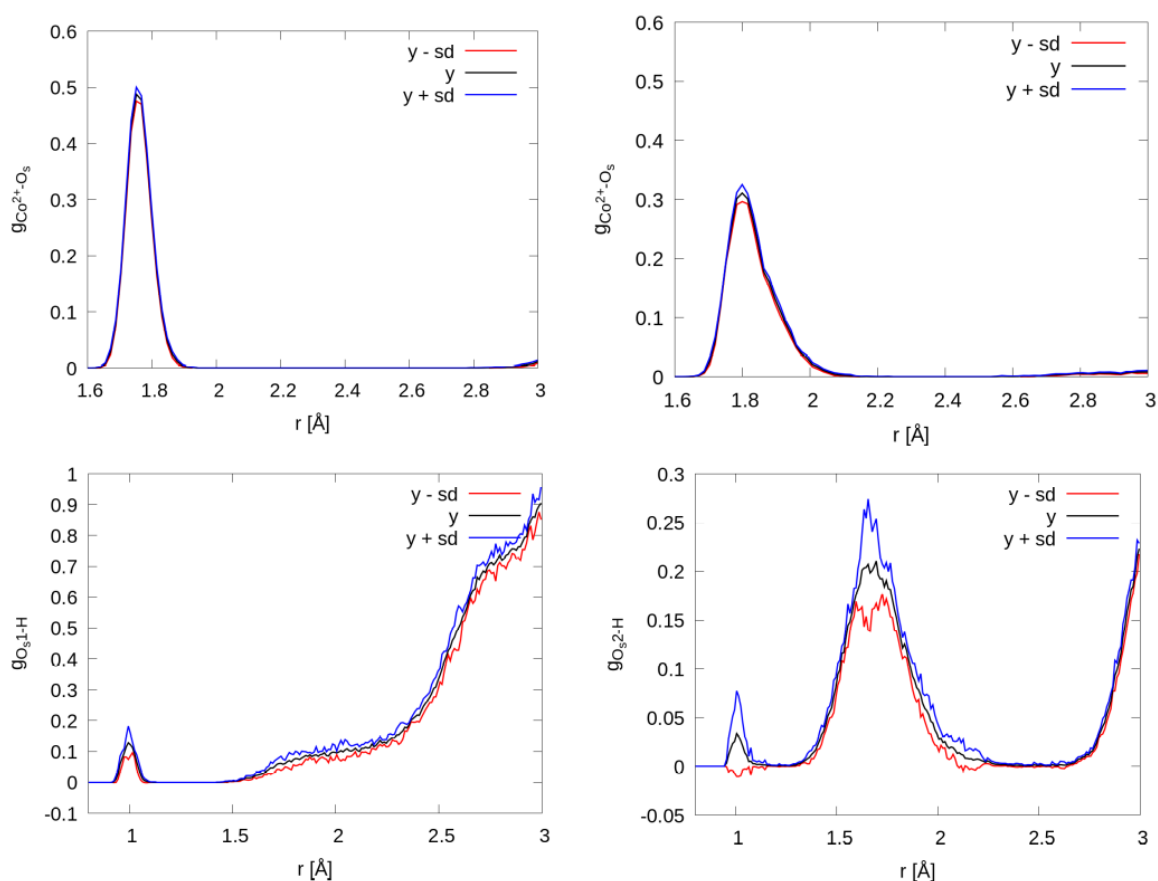


Figure S4: Average value of the radial distribution functions reported together with their standard deviation (sd), of the Co^{2+} to surface oxygens O_s distances, on the clean (top left) and water covered (top right) on the A-terminated surface. Corresponding values for the surface oxygens to water hydrogens (bottom).

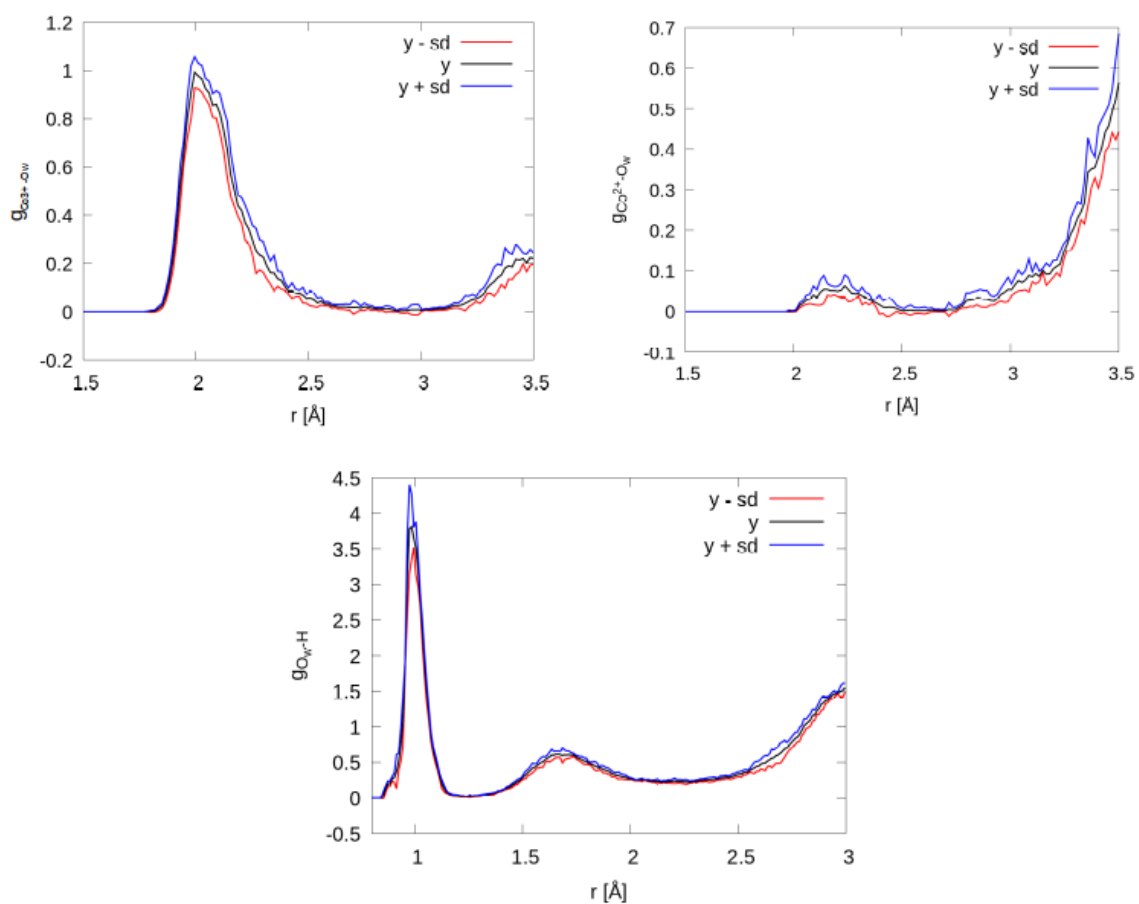


Figure S5: Average value of the radial distribution functions reported together with the standard deviation (sd), of the Co^{3+} to water oxygens O_w distances (left); of the Co^{2+} to water oxygens O_w distances (right) and of the water oxygens to water hydrogens distances (bottom), on the B-terminated surface.

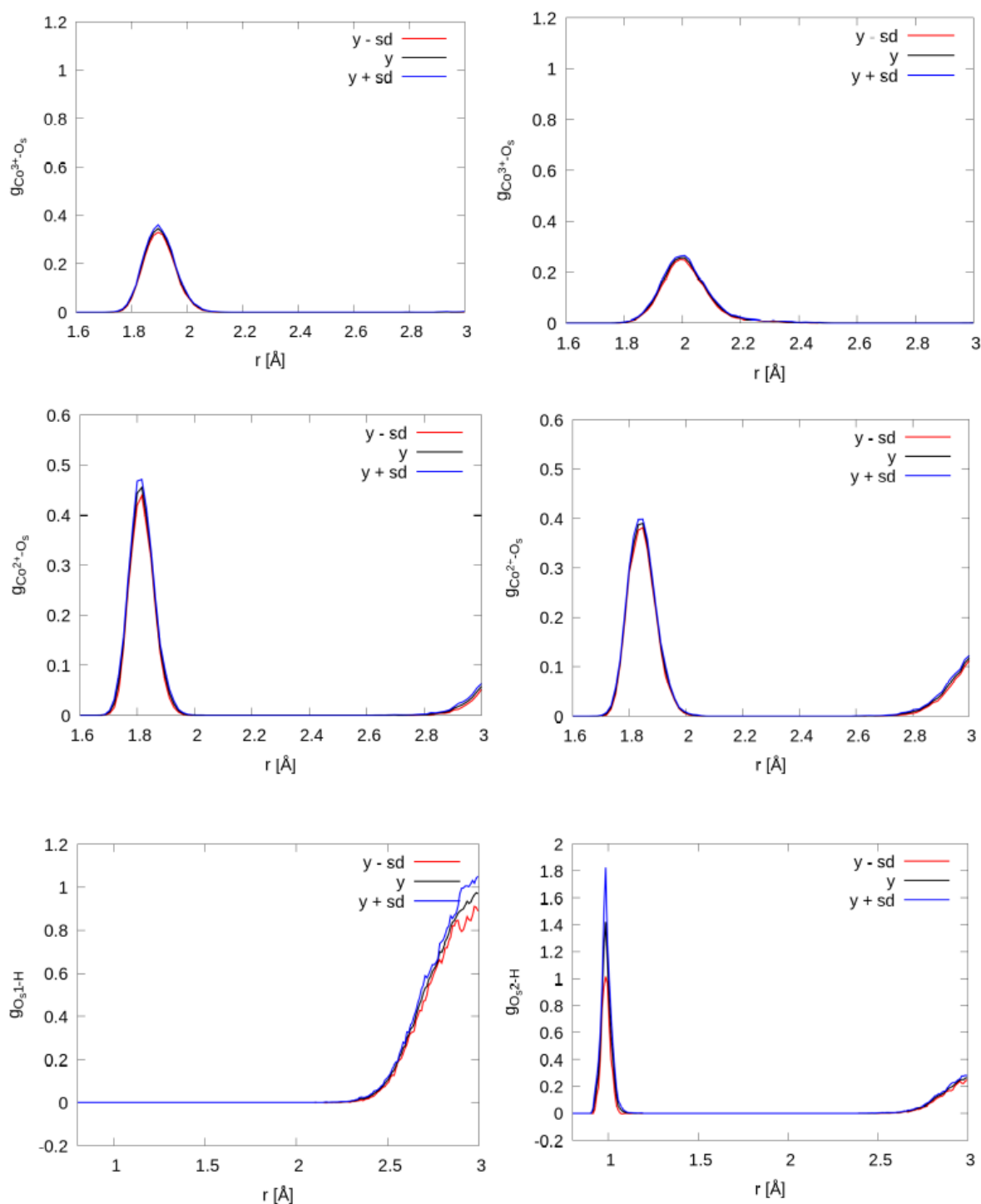


Figure S6: Average value of the radial distribution functions reported together with their standard deviation (sd), of the Co^{3+} to surface oxygens O_s distances on the clean (top left) and water covered (top right) B-terminated surface; for the Co^{2+} to surface oxygens O_s distances (middle left and right). Corresponding values for the surface oxygens to water hydrogens (bottom).