Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary materials for "Defect structures of the $Cr_2O_3(11\bar{2}0)$ surface: Effect of electron beam irradiation"

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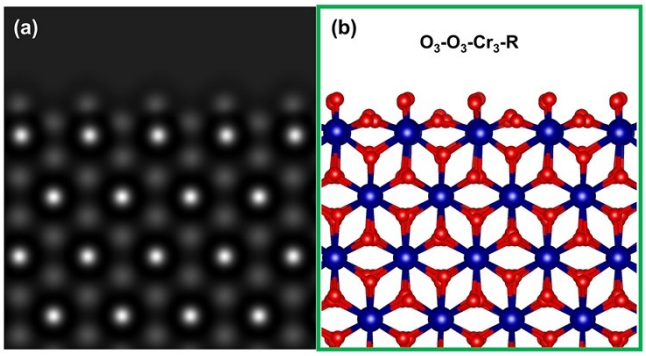

Fig. S1. (a) The simulated image and (b) atomic models of O_3-O_3-Cr_4-R termination relaxed by DFT calculations. The big and small balls are Cr and O atoms, respectively.

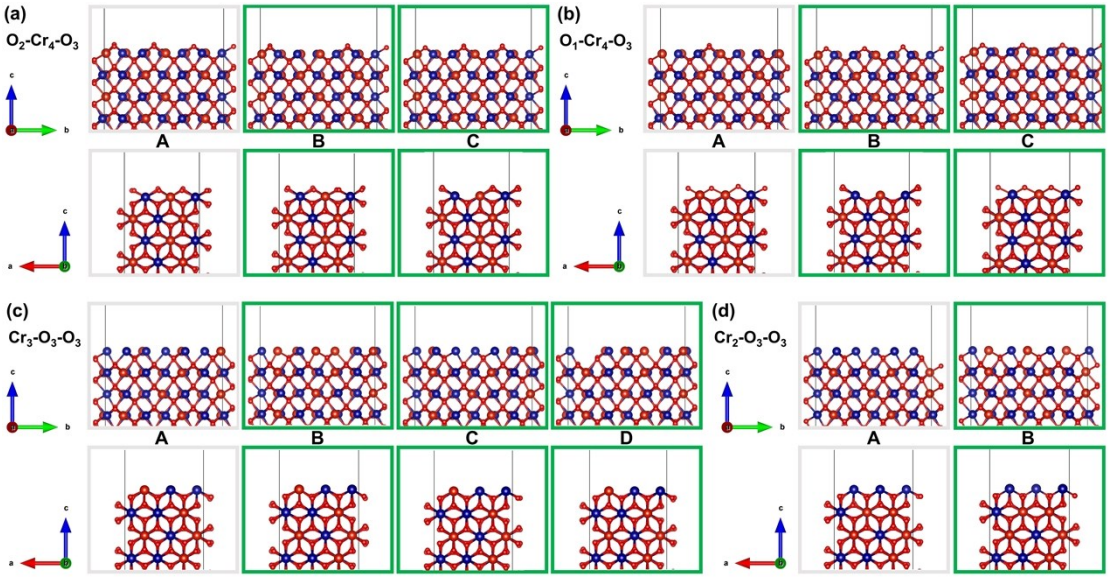

Fig. S2. The models of (a) O_2-Cr_4-O_3, (b) O_1-Cr_4-O_3, (c) Cr_3-O_3-O_3, and (d) Cr_2-O_3-O_3 structures with O or Cr atoms vacancies in different positions unrelaxed by DFT calculations. The big and

small balls are Cr and O atoms, respectively. The big balls with blue and orange represent spin parallel and anti-parallel with the (0001) plane. Models A represent the most stable structures.

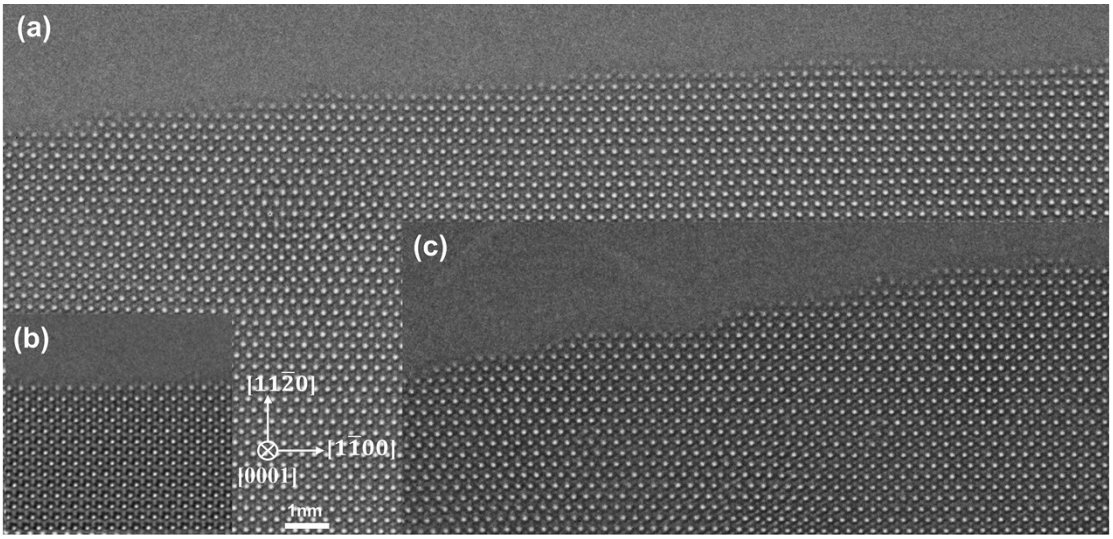

Fig. S3. The original aberration-corrected TEM images of the $Cr_2O_3(11\bar{2}0)$ surface, viewed along the [0001] zone axis.