

Supplementary Materials (SM) for
Functionalized ceria-niobium supported nickel catalysts for gas phase semi-
hydrogenation of phenylacetylene to styrene

Toyin Shittu¹, Abbas Khaleel², Kyriaki Polychronopoulou^{3,4} Mohammednoor Altarawneh^{1*},

¹Department of Chemical and Petroleum Engineering, United Arab Emirates University,
Sheikh Khalifa Bin Zayed Street, Al-Ain, 15551, United Arab Emirates

²Department of Chemistry, United Arab Emirates University,
Sheikh Khalifa Bin Zayed Street, Al-Ain, 15551, United Arab Emirates

³Center for Catalysts and Separation, Khalifa University of Science and Technology, Abu
Dhabi, P.O. Box 127788, United Arab Emirates.

⁴Department of Mechanical Engineering, Khalifa University of Science and Technology, Abu
Dhabi, P.O. Box 127788, United Arab Emirates

*Corresponding author's Email: mn.altarawneh@uaeu.ac.ae

Content List

Table S1. Rate of reaction and rate constant for stand-alone cerium (IV) oxide and the supported catalysts in phenylacetylene hydrogenation at 300 °C.

Figure S1. TGA result for the calcined catalysts

Figure S2. Pore size distribution of the prepared samples, CeO₂ (a); Nb₂O₅ (b); 6%Ni-Ce (c); 5%Ni-Ce (d); Ni-10%NbCe (e); and Ni-5%NbCe (f).

Figure S3. FTIR spectra of the pure and prepared samples.

Figure S4. SEM image of; , CeO₂ (a); Nb₂O₅ (b); 6%Ni-Ce (c); 5%Ni-Ce (d); Ni-10%NbCe (e); and Ni-5%NbCe (f).

Figure S5. EDS profile of the prepared samples, CeO₂ (a); Nb₂O₅ (b); 6%Ni-Ce (c); 5%Ni-Ce (d); Ni-10%NbCe (e); and Ni-5%NbCe (f).

Figure S6. XRD plot of the spent catalysts

Figure S7. Optimized geometries for the four considered Ni/Nb-ceria decorated surfaces.

Table .S1. Rate of reaction and rate constant for stand-alone cerium (IV) oxide and the supported catalysts in phenylacetylene hydrogenation at 300 °C.

Catalysts	Reaction rate ($\text{mol}\cdot\text{s}^{-1}\cdot\text{g}^{-1}_{\text{cat}}$)	Rate constant, k ($\text{L}\cdot\text{s}^{-1}\cdot\text{g}^{-1}_{\text{cat}}$)
CeO_2	0	0
6NiCe	4.781×10^{-6}	8.441×10^{-7}
5NiCe	7.715×10^{-6}	2.173×10^{-6}
Ni-5%NbCe	8.896×10^{-6}	3.294×10^{-6}
Ni-10%NbCe	2.945×10^{-6}	4.217×10^{-7}

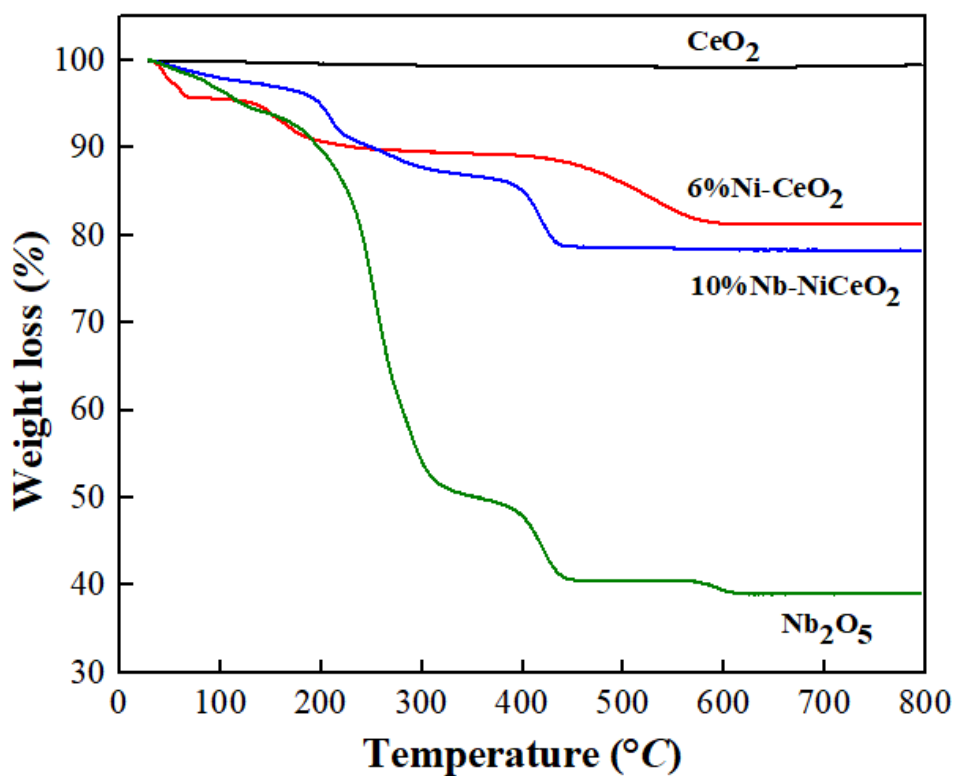


Fig. S1. TGA result for the calcined catalysts

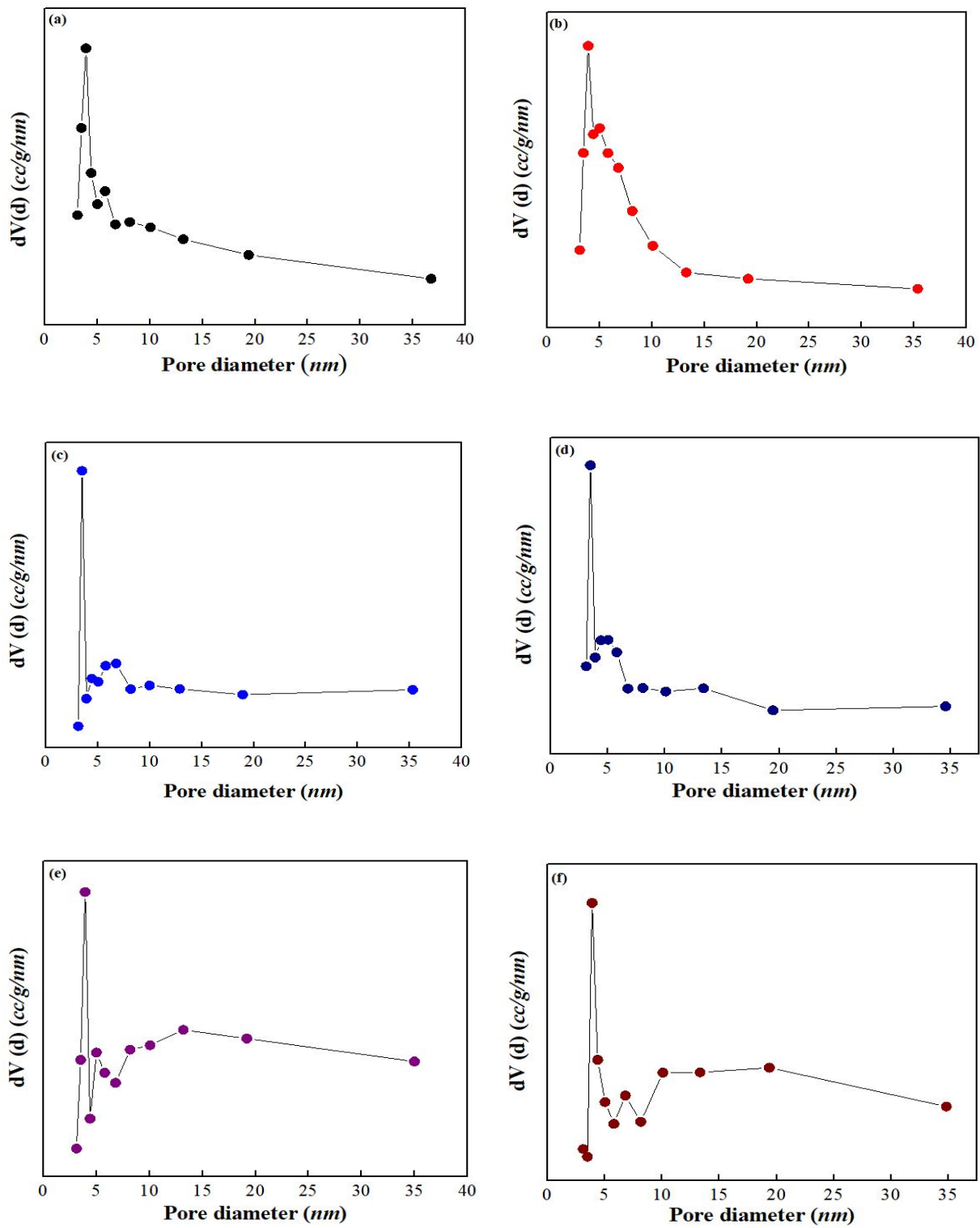


Fig. S2 Pore size distribution of the prepared samples, CeO_2 (a); Nb_2O_5 (b); 6%Ni-Ce (c); 5%Ni-Ce (d); Ni-10%NbCe (e); and 5%Ni-NbCe (f).

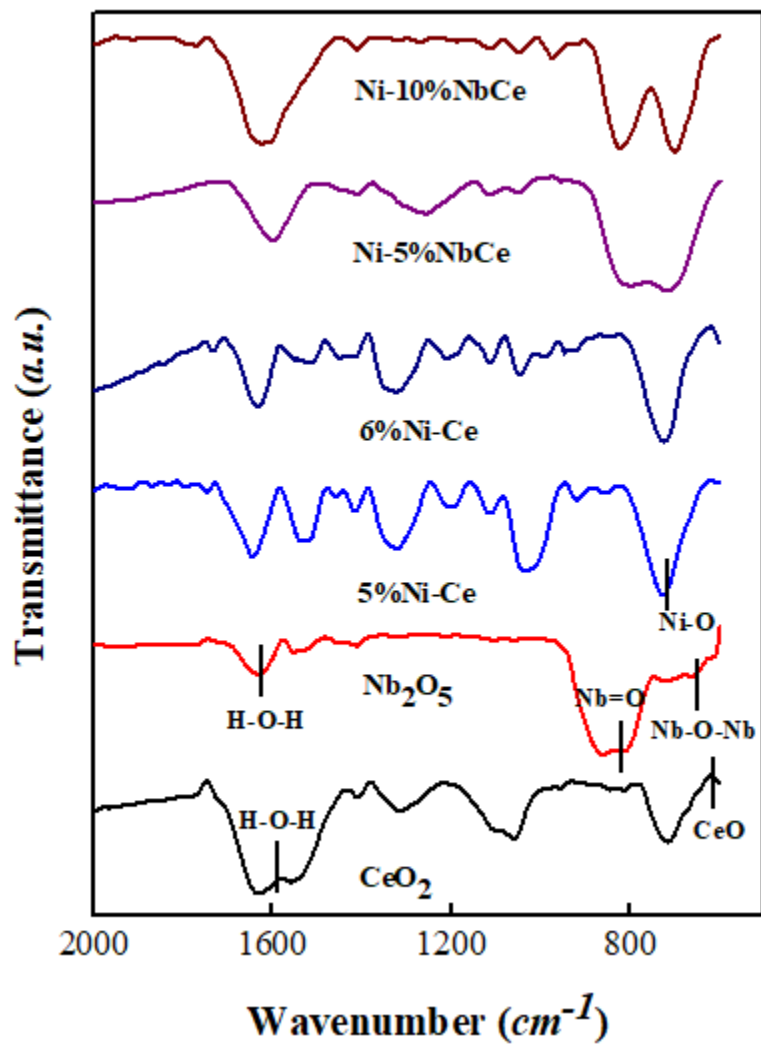


Fig. S3. FTIR spectra of the pure and prepared samples.

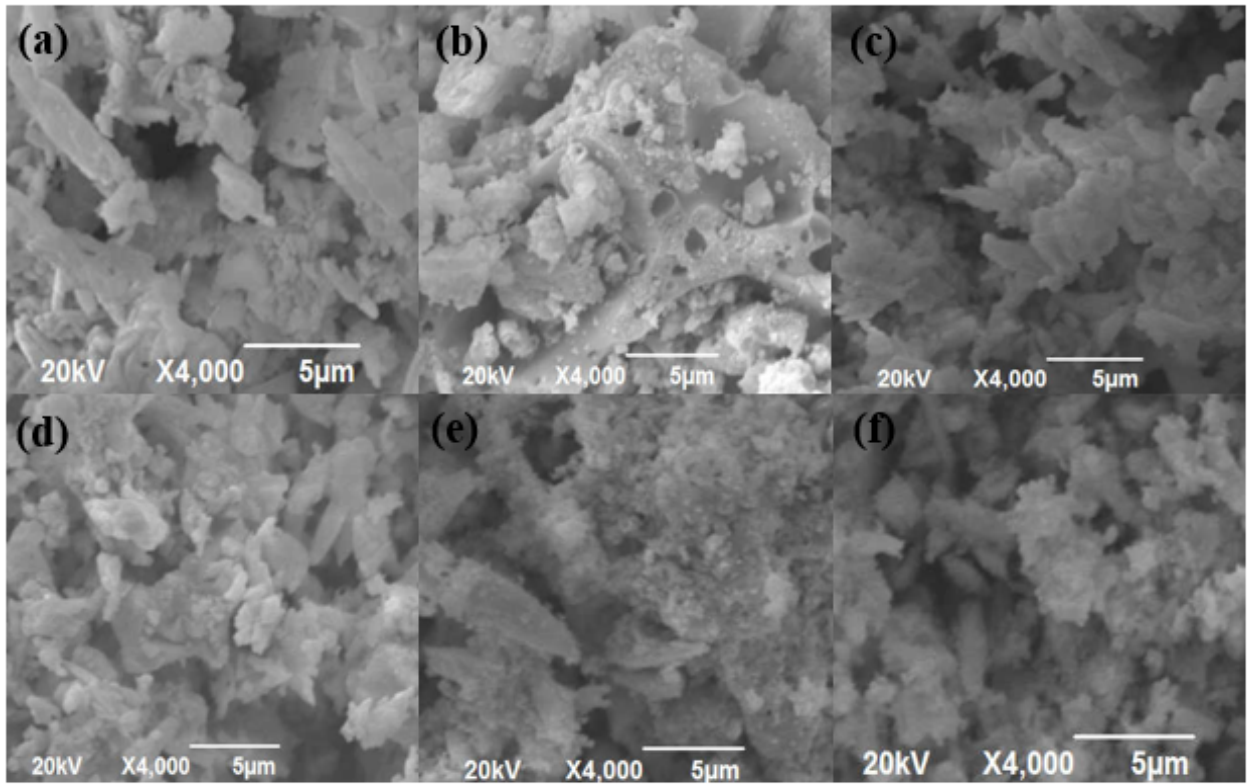
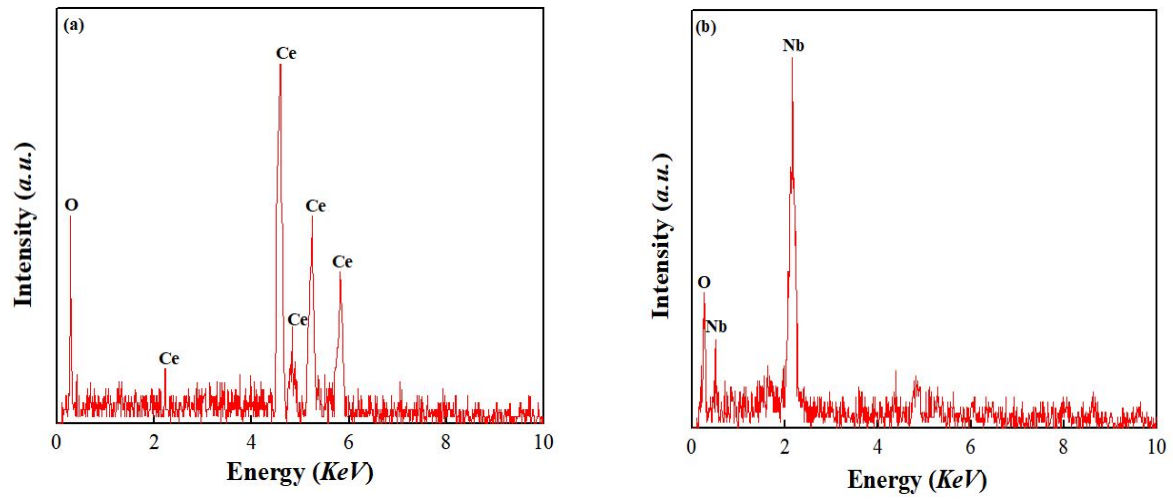


Fig. S4. SEM image of; CeO₂ (a); Nb₂O₅ (b); 6%Ni-Ce (c); 5%Ni-Ce (d); Ni-10%NbCe (e); and Ni-5%NbCe (f).



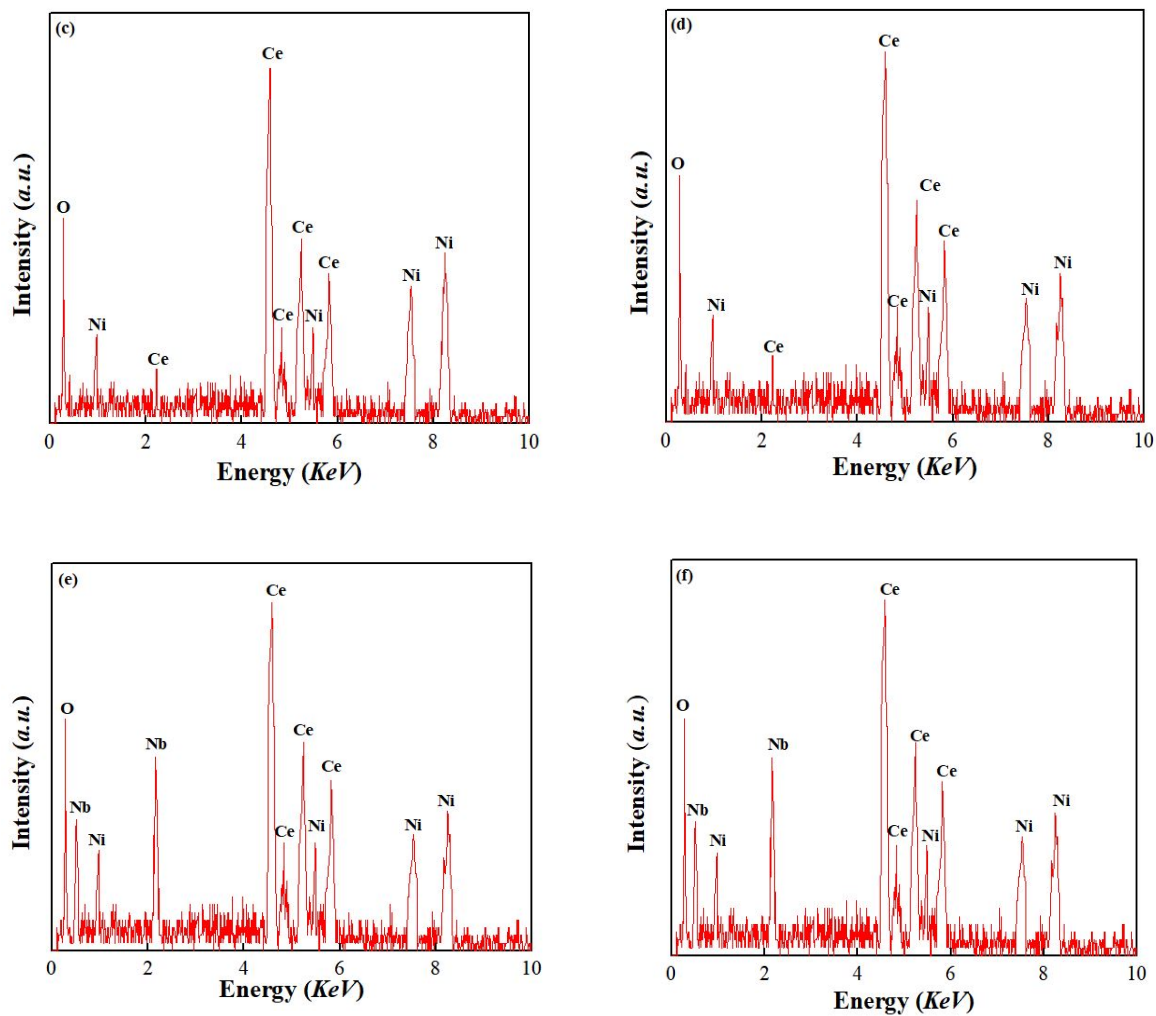


Fig. S5. EDS profile of the prepared samples, CeO_2 (a); Nb_2O_5 (b); 6%Ni-Ce (c); 5%Ni- Ce (d); Ni-10%NbCe (e); and Ni-5%NbCe (f).

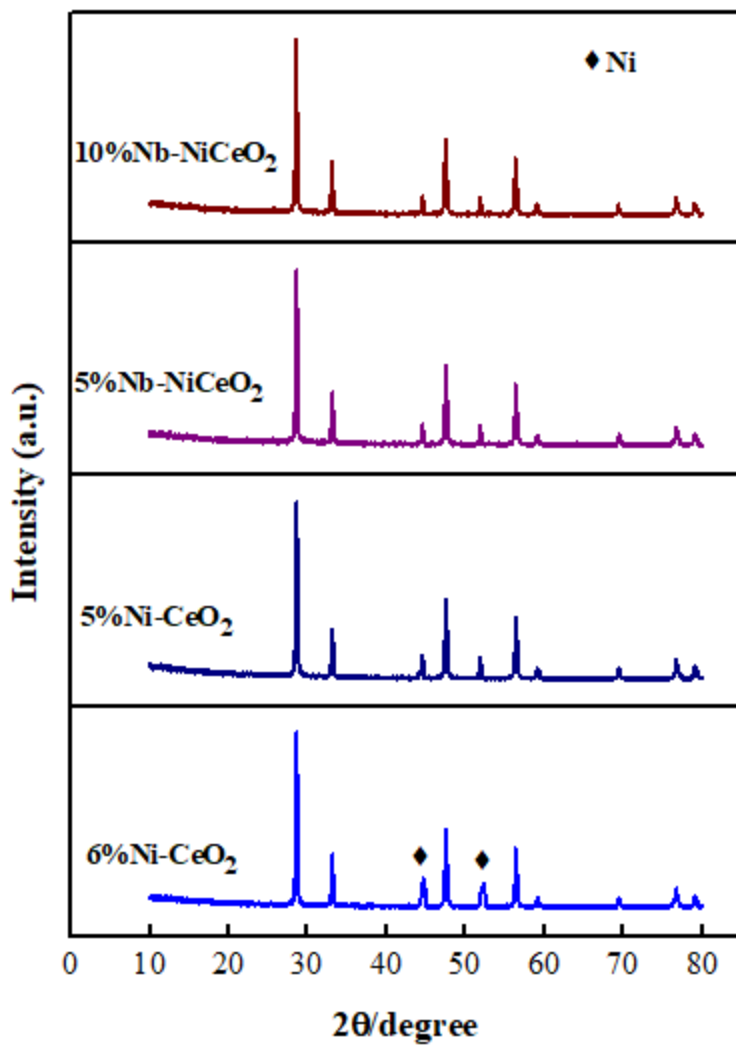


Fig. S6. XRD plot of the spent catalysts

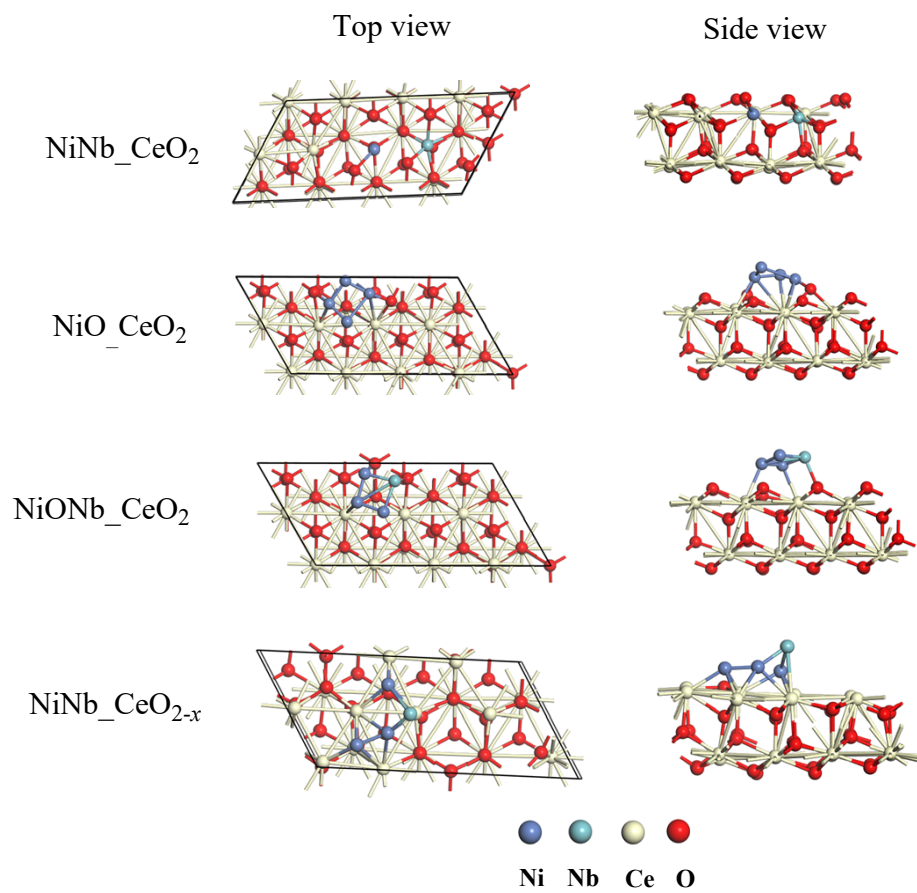


Fig. S7. Optimized geometries for the four considered Ni/Nb-ceria decorated surfaces.