Supporting information

High Electrocatalytic Performance Inspired by Crystalline/Amorphous Interface in PtPb Nanoplate

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Figures

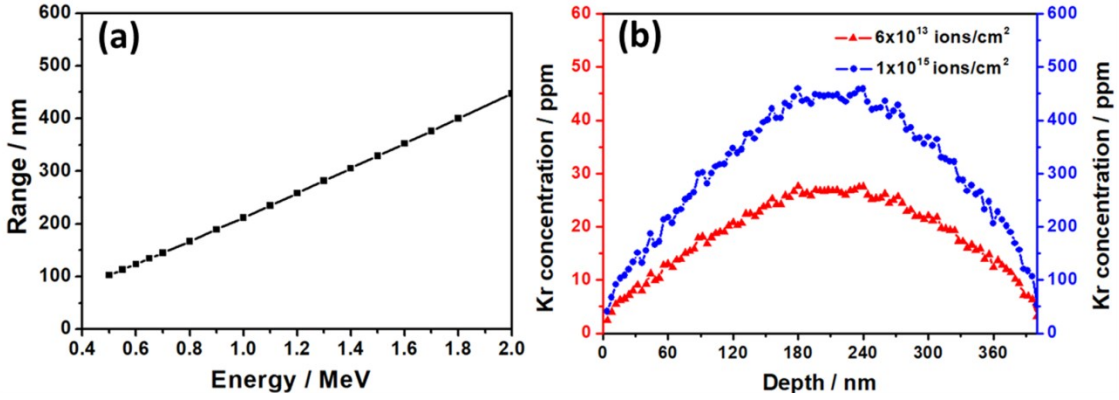


Fig. S1. (a) Relationship between the range and energy of Kr^{3+} ions. (b) The depth profile of Kr concentration obtained from SRIM simulation of PtPb subjected to Kr^{3+} ion irradiation at 1 MeV with a total fluence of 6×10^{13} ions/cm^2 and 1×10^{15} ions/cm^2.

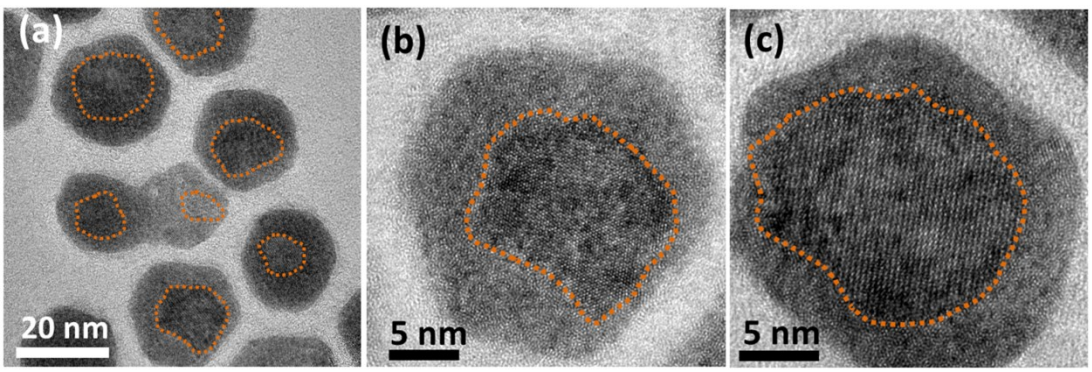


Fig. S2. TEM images of PtPb NP samples irradiated by Kr ions with dose of

$6 \times 10^{13}\ ions \cdot cm^{-2}$. (a) Overview TEM image containing multiple ion-irradiated PtPb NPs. (b)-(c) TEM images of typical ion-irradiated PtPb NPs. The PtPb NPs contain crystalline phase and amorphous phase simultaneously, and the crystalline region is surrounded by the amorphous region to form interface. The interface of crystalline phase and amorphous phase are marked by dotted line.

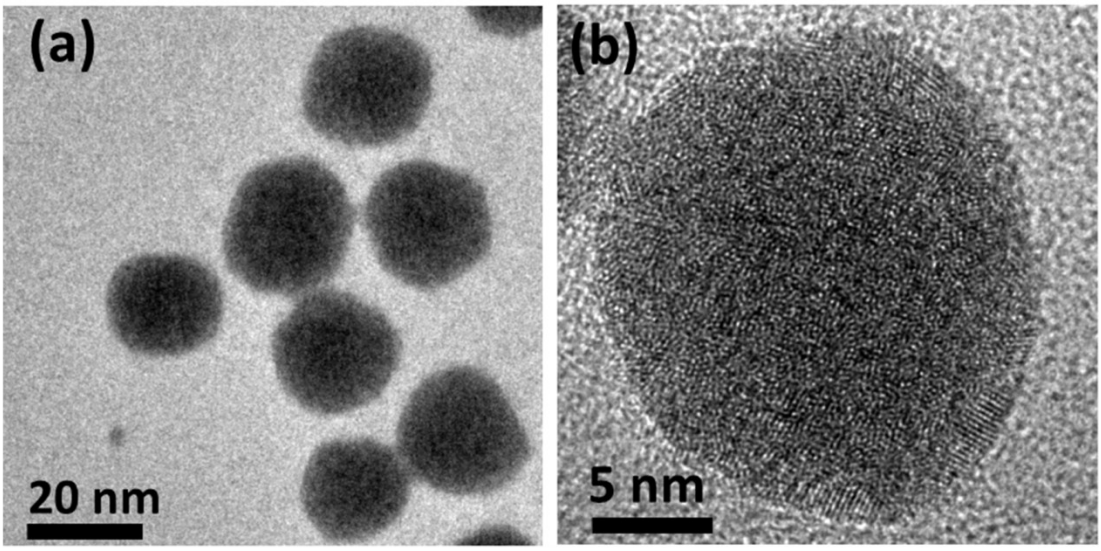


Fig. S3. TEM images of PtPb NP samples irradiated by Kr ions with dose of $1 \times 10^{15}\ ions \cdot cm^{-2}$. (a) Overview TEM image containing multiple ion-irradiated PtPb NPs. (b) TEM image of typical ion-irradiated PtPb NP. The PtPb NPs are almost amorphous

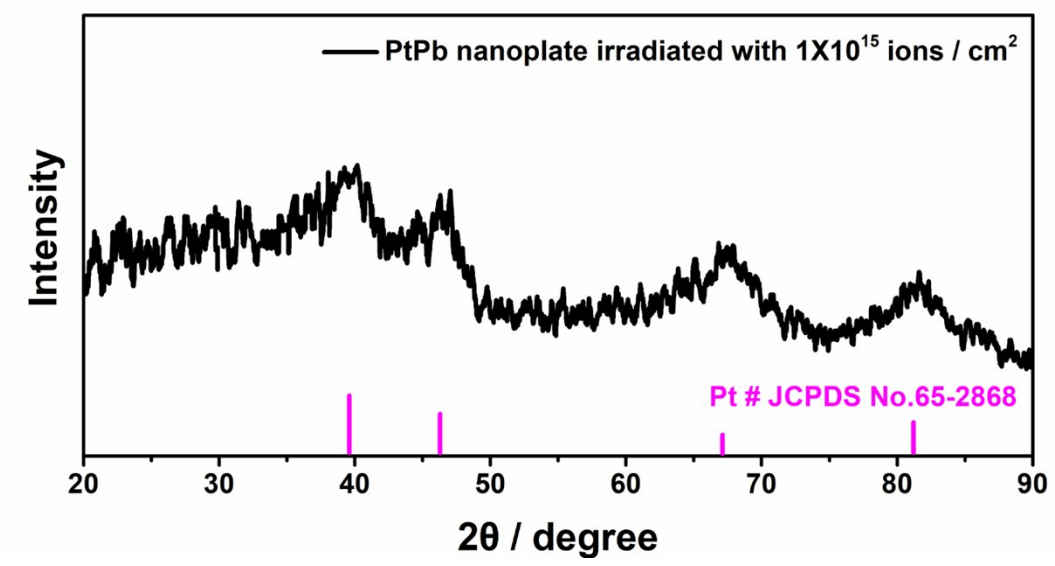


Fig. S4. PXRD patterns of PtPb NPs irradiated with the dose of $1 \times 10^{15}\ ions \cdot cm^{-2}$.

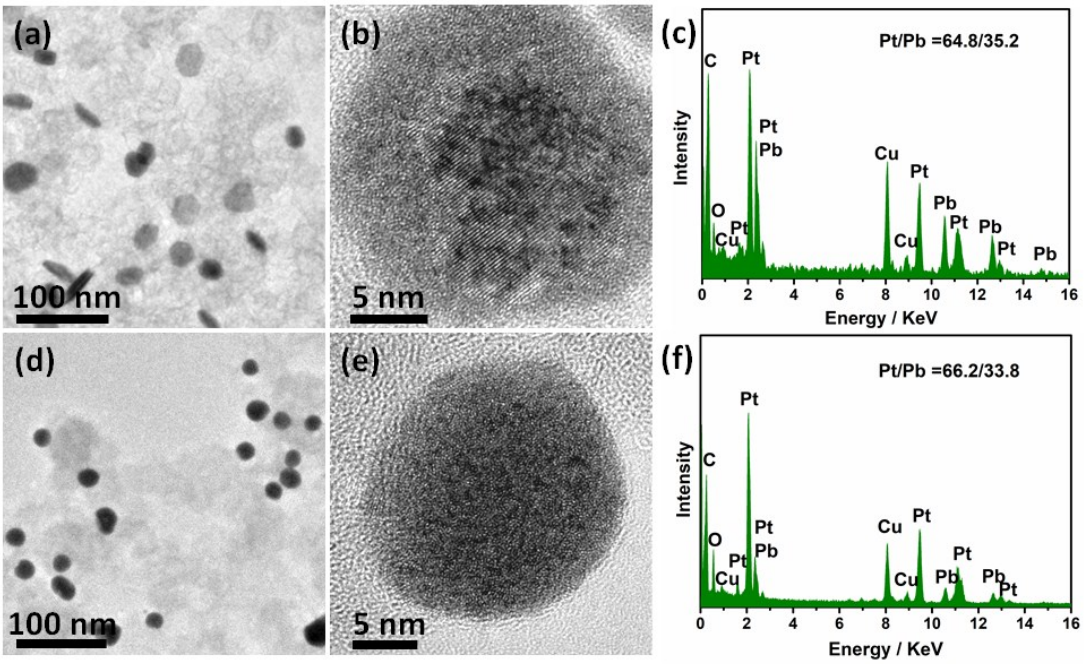


Fig. S5. (a) TEM and (b) HRTEM images of PtPb-CA /C NPs after electrochemical tests. (c) EDS result of after-electrochemical-tests PtPb-CA /C NPs showing that the atomic ratio (Pt:Pb) is 64.8/35.2. (d) TEM and (e) HRTEM images of PtPb-A /C NPs after electrochemical tests. (f) EDS result of after-electrochemical-tests PtPb-A /C NPs showing that the atomic ratio (Pt:Pb) is 66.2/33.8.

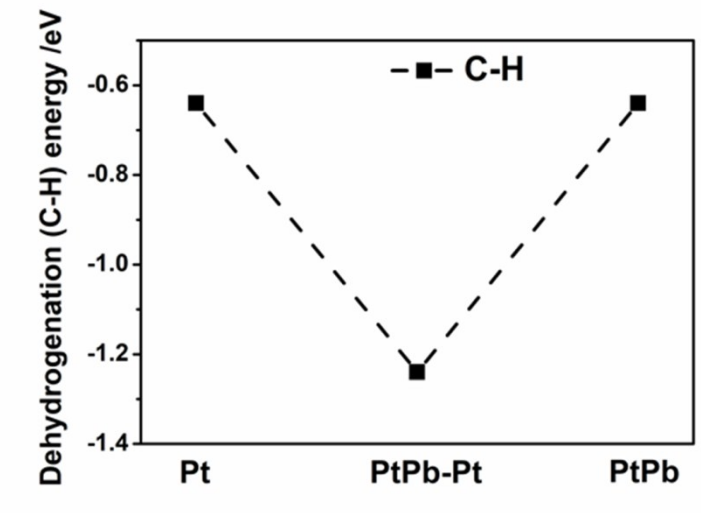


Fig. S6. Dehydrogenation energy in MOR represented by $CH_3O^* \rightarrow CH_2O^* + H^*$ (breaking C-H bond) in Pt surface, PtPb-Pt interface (C/A interface) and PtPb surface.

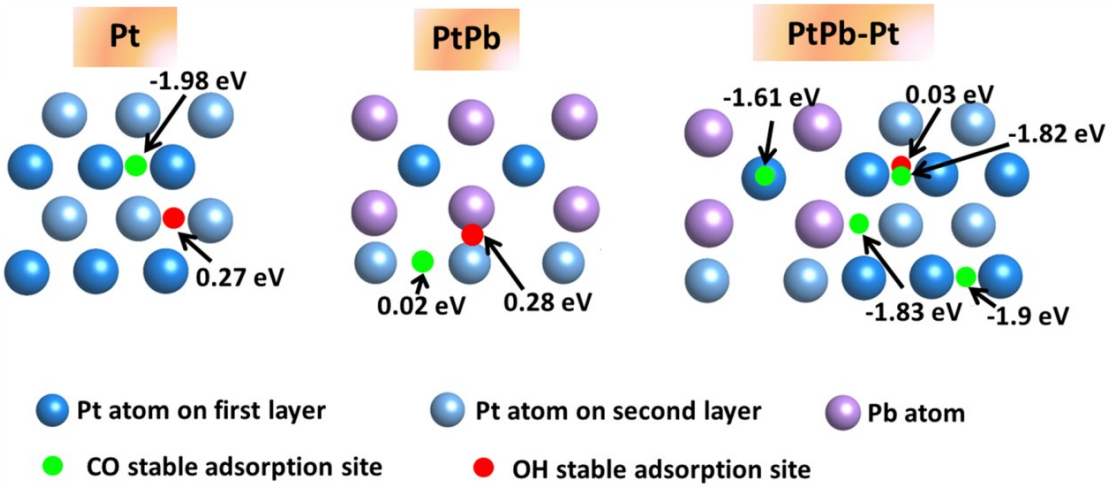
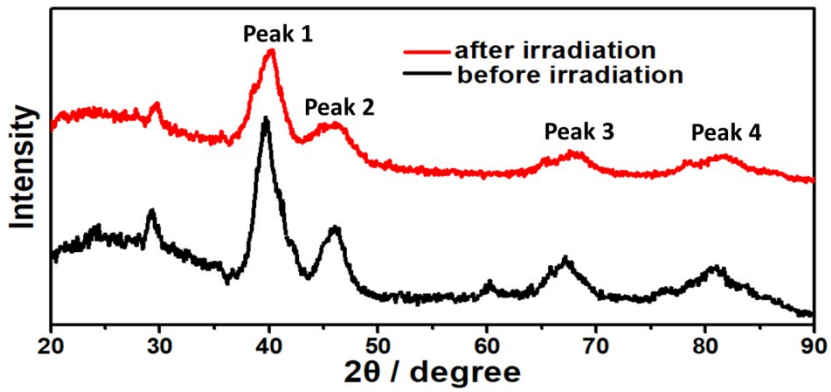


Fig. S7. The model of Pt surface, intermetallic PtPb surface and interface of PtPb-Pt (C/A interface) for DFT simulation. The most stable CO and OH adsorptions on different sites were screened and the adsorption energy on these three kinds of surface is labeled in the schematic.

Tables

Table S1. The full width at half maximum (FWHM) of PtPb NPs before and after ion irradiation from PXRD spectrum.



Peak number	FWHM of NPs before ion irradiation / degree	FWHM of NPs after ion irradiation / degree
1	2.78	3.02
2	3.28	4.04
3	3.91	5.44

4	6.05	6.76

Table S2. MOR activities of different catalysts. MOR measurements were performed in 0.1 M $HClO_4$+0.1 M methanol at a scan rate of 50 mV /s.

Catalyst	Specific activity (mA/cm^2_{Pt})	Mass activity (A/mg_{Pt})
Pt /C	0.78	0.36
PtPb /C	2.30	0.96
PtPb-CA /C	4.32	1.31
PtPb-A /C	1.76	0.77

Table S3. Dehydrogenation reaction energy (ΔE) of intermediates in Pt surface, PtPb-Pt interface (C/A interface) and PtPb surface in MOR. The ΔE of deep dehydrogenation steps on Pt surface and PtPb-Pt interface were further compared to see the thermal stability differences.

Reaction	Reaction energy (eV)		
	Pt	PtPb-Pt (C/A interface)	PtPb
$CH_3OH \rightarrow CH_2OH$	-0.62	-0.77	-0.35
$CH_2OH \rightarrow CH_2O$	-0.21	-0.42	-0.04
$CH_3OH \rightarrow CH_3O$	-0.19	0.17	0.25
$CH_3O \rightarrow CH_2O$	-0.64	-1.24	-0.64
$CH_2OH \rightarrow CHOH$	-0.23	0.14	-
$CH_2O \rightarrow CHO$	-0.60	-0.82	-
$CHOH \rightarrow COH$	-0.83	0.66	-
$COH \rightarrow CO$	-0.95	-1.06	-

Table S4. CO and OH adsorption energy of atoms in Pt surface, PtPb-Pt interface (C/A interface) and PtPb surface.

Adsorbate	Adsorption energy (eV)		
	Pt	PtPb-Pt (C/A interface)	PtPb
CO	-1.98	-1.61	0.02
OH	0.27	0.03	0.28