Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2018

Electronic Supplementary Information

Dipole moment driven diesel soot oxidation over alkali metal chlorides

Hui Chen,[a] Yexin Zhang*[ab] and Jian Zhang*[ab]

[a.] *Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, 1219 Zhongguan West Road, Ningbo 315201, People's Republic of China.*

[b.] *University of Chinese Academy of Sciences, 19A Yuquan Road, Beijing 100049, People's Republic of China.*

*Correspondence author: Yexin Zhang, zhangyexin@nimte.ac.cn; Jian Zhang, jzhang@nimte.ac.cn

Experimental

Printex-U from Degussa was used as model soot and was mixed with some alkali metal chlorides (AM-Cl) model catalysts, including NaCl, KCl, RbCl and CsCl. A full contact condition between soot and catalysts were achieved by direct incipient wetness impregnation of the soot powder with aqueous solutions of catalysts. After impregnation, the samples were dried overnight at 100 °C. For the convenience to compare the intrinsic activities of AM, the atomic ratio of AM/C was kept to be 2:1 for all soot-catalyst mixtures.

A temperature programmed oxidation (TPO) test was conducted to evaluate the activity of catalyst. The soot-catalyst mixture containing 5 mg soot was packed by silica in a fixed-bed micro reactor. A gas flow with 10 vol.% O_2 in N_2 was introduced at a flow rate of 50 mL/min at room temperature and then the TPO was started at a heating rate of 2 °C/min until 650 °C. The products of CO_2 and CO in the effluent were online detected by an infrared gas analyzer (Talantek TY9000). The activities of the catalysts were evaluated by the characteristic temperature (T_x) of soot oxidation, which is defined as the temperature at which x% of the soot is burned. The selectivity to CO_2 formation (S_{CO2}) is defined as the accumulated amount of CO_2 production as percentage of the sum amount of CO_2 and CO products.

X-ray photoelectron spectroscopy (XPS) characterizations were carried out on AXIS ULTRADLD Multifunctional X-ray Photoelectron Spectroscope with an Al Kα radiation source at room temperature and under a vacuum of 10^{-7} Pa (10^{-9} Torr). The starting angel of the photoelectron was set at 90°. The spectrum was calibrated with a C1s spectrum of 284.6 eV. The Raman spectra were collected with a Renishawin Via-reflex spectrometer using back-scattered light from a 532 nm laser focused through a 50×objective lens.

Supporting Figures

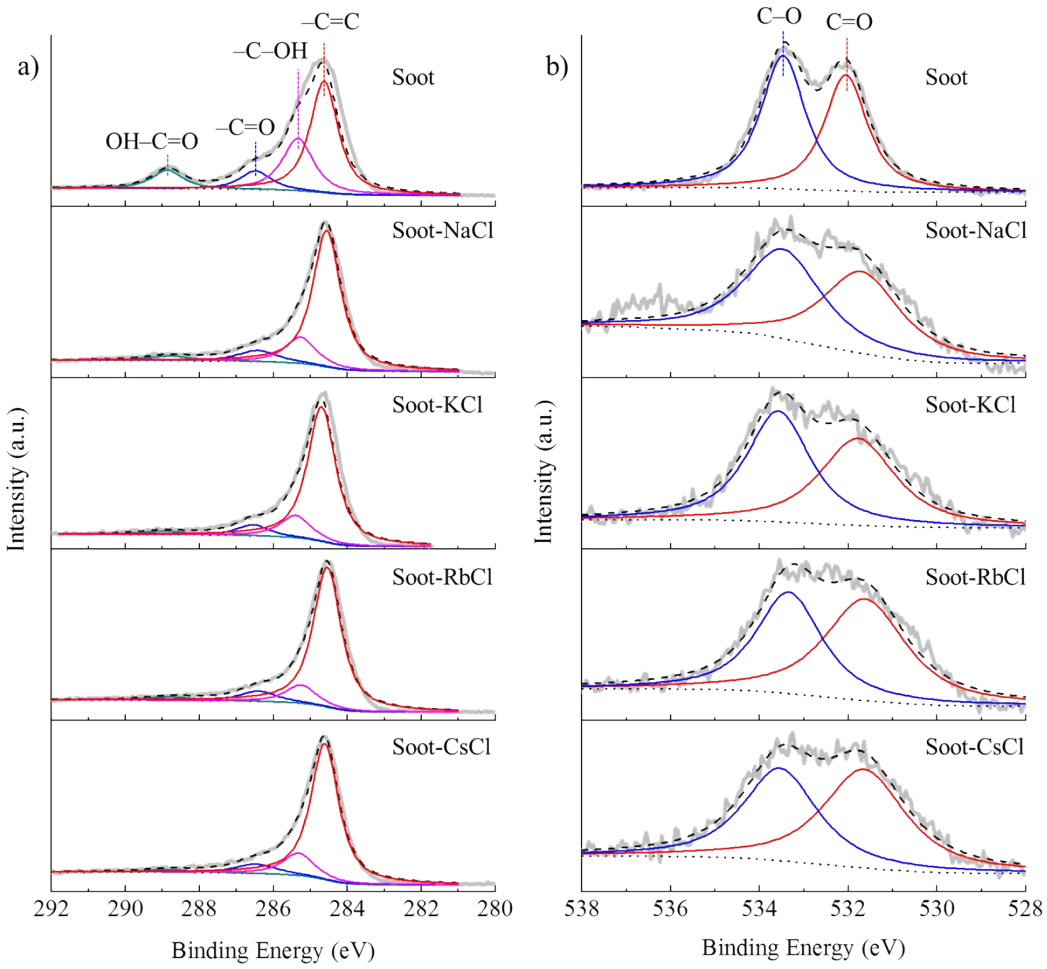

Fig. S1 C 1s (a) and O 1s (b) XPS spectra as well as the corresponding deconvolutions for the bare soot and the soot-catalyst mixtures after the soot conversion of 50%

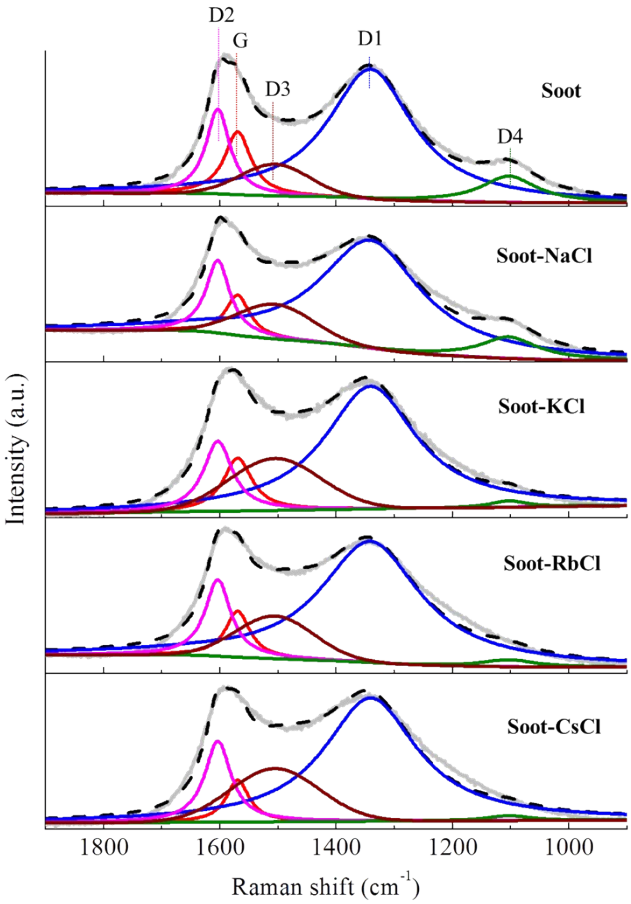

Fig. S2 Raman spectra and corresponding deconvolutions of the bare soot and the soot-catalyst mixtures after the soot conversion of 50%

Supporting Tables

Table S1 Characteristic parameters of soot oxidation with and without AM-Cl catalysts

Sample	T_5 (°C)	T_{10} (°C)	T_{50} (°C)	S_{CO2} (%)
Soot	469.6	504.4	593.1	45.6
Soot-NaCl	421.1	443.6	489.7	86.7
Soot-KCl	401.3	425.4	472.4	86.7
Soot-RbCl	350.4	366.8	419.9	93.2
Soot-CsCl	374.7	391.2	434.5	93.3

Table S2 Fractions of functional groups based on the deconvolutions of C1s spectra and $I_{C–O}/I_{C=O}$ ratios based on O1s spectra as well as the O/C atomic ratios for the bare soot and the soot-catalyst mixtures after the soot conversion of 50%.

Sample	OH–C=O (%)	–C=O (%)	–C–OH (%)	C=C (%)	$I_{C–O}/I_{C=O}$	O/C
Soot	8.74	9.31	27.79	54.15	1.18	0.188
Soot-NaCl	6.93	9.24	9.39	74.44	1.08	0.115
Soot-KCl	2.65	5.00	8.12	84.23	0.93	0.090
Soot-RbCl	6.95	9.57	18.76	64.72	0.80	0.072
Soot-CsCl	4.98	6.53	11.43	77.06	0.83	0.082