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Structure-based drug design

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Our research is to solve structures of PPAR, a key molecular target of type II diabetes, in complex with novel agonists discovered and developed in our division and consequently these structures could provide insight on how to design compounds with more potency. Crystals of PPAR were soaked into solution containing compound SP990 and compound SP999. These crystals diffract to around 3Å in Spring8 station SP12B2. All dataset, including one PPAR native dataset and three PPAR complex datasets, were collected on a CCD detector. The data collection parameters for these datasets are summarized in table 1. All datasets have been processed by HKL2000 in station SP12B2. The data process results are shown in table2. After data process, it has been found the distance should be corrected to 143mm, 172mm, 152mm, and 182mm for datasets of PPAR native , PPAR with SP990, PPAR with SP999[a] and PPAR with SP999[b], respectively. This result indicates the distance of CCD detector in station SP12B2 requires adjustment

Table 1. The summary of data collection parameters

Sample	Distance (mm)	Wavelength (Å)	Oscillation range(X)	Beam position (x,y)	Exposure time (sec)	Total frames
PPAR native	140	1.1	1	(94.32, 93.76)	60	134
PPAR with SP990	170	1.1	1	(94.32, 93.76)	60	208
PPAR with SP999[a]	150	1.1	1	(94.32, 93.76)	60	200
PPAR with SP999[b]	180	1.1	1	(94.32, 93.76)	60	133

Table 2 . The summary of data process results

Data collection statistics	PPARnative	PPAR with SP990	PPAR with SP999[a]	PPAR with SP999[b]
Space group, C2 ($\alpha=\gamma=90°$)	a=92.365 b=61.816 c=118.456 β=102.840	a=92.458 b=61.889 c=118.340 β=102.64	a=92.547 b=61.740 c=118.132 β=102.882	a=92.328 b=61.727 c=118.103 β=102.882
Resolution range(Å)	50.0-3.0	30.0-2.9	25.0-3.5	30.0-3.0
Completeness(%)	91.4	94.7	98.5	93.1
R_{merge}(%)	6.3	7.9	9.1	7.3
I/σ(I)	14.75	11.5	5.72	7.47

C03B12XU-1500N BL12XU

Resonant Inelastic X-ray Scattering of NiO, CoO and Related Materials

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Understanding the nature of high T_c superconductivity of Cu oxides is one of most important subject in condensed matter physics. The existence of layered CuO_2 plane is recognized as crucial for its high T_c property. Layered Co compound $NaCo_2O_4$ is known to exhibit large thermopower. The material has layer CoO_2 plane and each layers are separated by Na atoms. Recently, $Na_{0.35}CoO_2 \cdot 1.3H_2O$ in which water molecules are intercalated between the CoO_2 layers was found to show superconductivity at T_c~5K. This compound has attracted a lot of interest due to its resemblance of superconducting Cu oxides.

The resonant inelastic x-ray scattering (RIXS) is a powerful technique which can probe electronic excitations in condensed matter. RIXS experiments have been carried out on various high T_c cuprates and provides its unique information on their electronic properties. Understanding the electronic properties of layered Co oxides is an important step toward understanding the nature of its superconductivity.

Polycrystalline sample of $Na_{0.7}CoO_2$ was made and characterized as described in Ref.[1]. The experiment was carried out at BL12XU at SPring8. The sample, analyzer and detector were maintained on Rowland circle condition for the RIXS experiment. Ge(444) 1m spherical bent analyzer was used. The total resolution was about 1.2eV.

Fig.1 shows (a) x-ray absorption spectra of CoO and $Na_{0.7}CoO_2$ and (b) RIXS spectra of $Na_{0.7}CoO_2$. Excitation energies for RIXS experiment are selected (a)~(f) from absorption spectrum. The three structures (A), (B) and (C) were observed about 5.3,7.1 and 10.7eV respectively. The structures (A) and (B) are assigned as ground state to $3d^{n+1}\underline{L}$, $\underline{L}$ denotes a hole state at the oxygen site. Since the high transferred energy of structure (C), this structure can be assigned as second charge transfer excitation $3d^{n+2}\underline{L}^2$, in which two holes at the oxygen site are involved. This excitation can be expected when the system has low spin ground state. This result is consistent with HE-PES experiment data [2]. Theoretical calculation is in progress to explain in detail the structures of the spectra.

[1] K. Takada , H. Sakurai, E. Takayama-Muromachi, F. Izumi, R. A. Dilanian, T. Sasaki Nature **53**, 422 (2003).
[2] A. Chainani et.al, cond-mat/ 0312293.

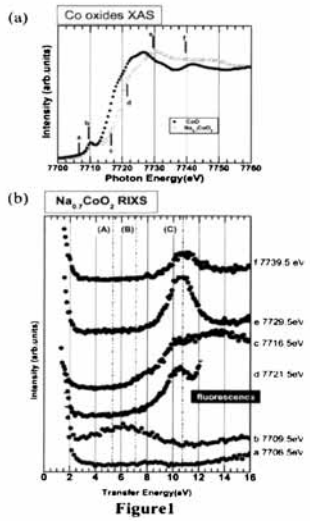

Figure1

Fig.1 (a) Co *K*-edge absorption spectra of $Na_{0.7}CoO_2$ and CoO. (b) RIXS spectra of $Na_{0.7}CoO_2$.