DNAフェルミ準位近傍の電子状態計測

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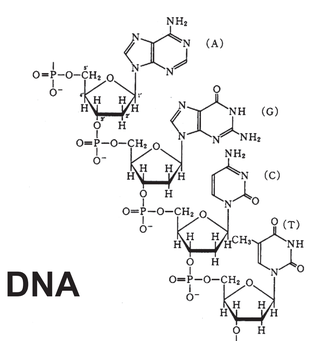
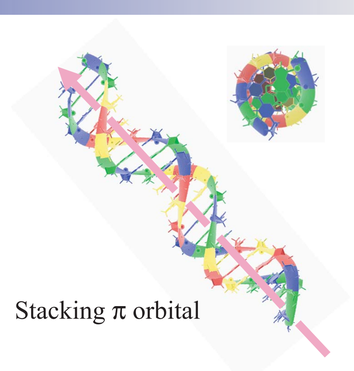
Characterization of DNA by Resonant Photoemission Spectroscopy

共同研究：　分子研　初井宇記、小杉信博
阪大産研　谷口正輝、川合知二

Introduction

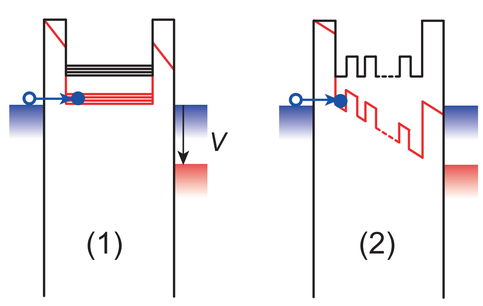


DNA



Stacking π orbital

A candidate for future molecular devices as wire



D. Porath et al., Nature 403, 635 (2000).

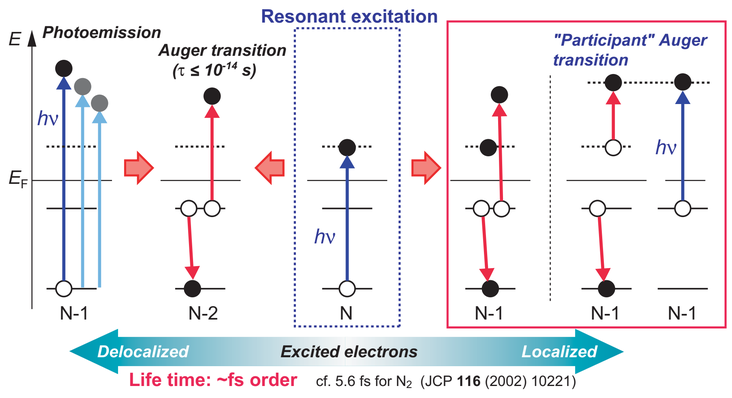
For DNA, two antithetical mechanisms have been proposed.

(1) Molecular band conduction (**delocalized**)

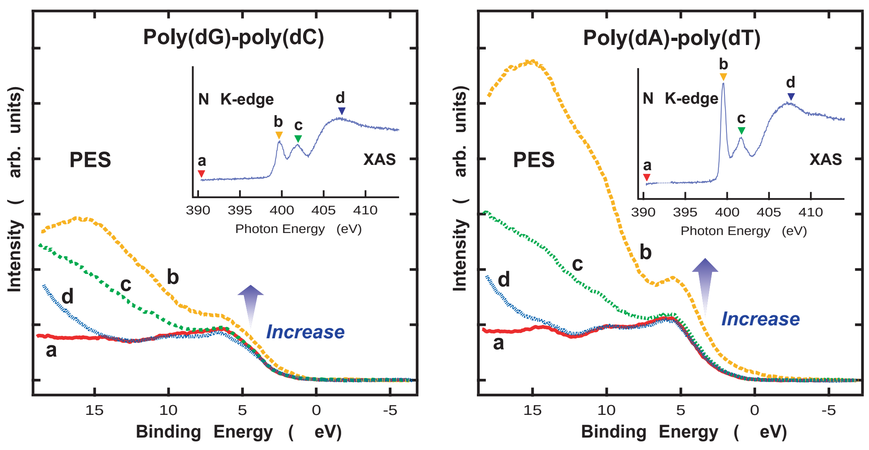
(2) Sequential hopping between **localized** bases

The experimental characterization of electronic structures near the Fermi level has been desired to clarify these conduction mechanisms.

Resonant excitation process

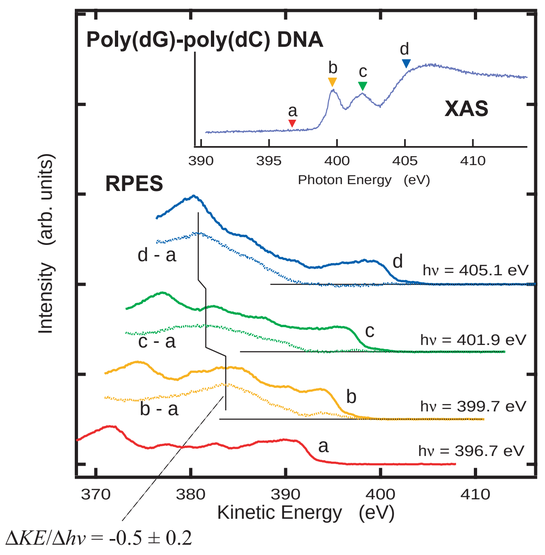


RPES near Fermi level

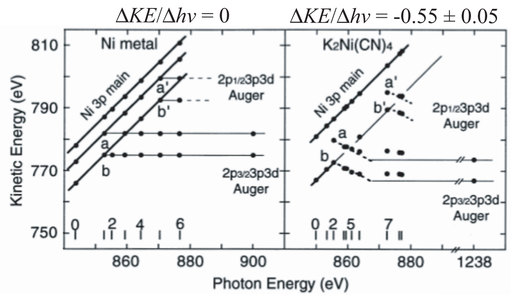


Excited electrons have a finite life time in the π state.*

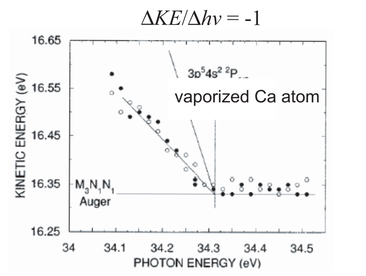
Auger electron component



Effect on kinetic energy of Auger electrons



Y. Takata et al., J. Electron Spectrosc. Relat. Phenom. 101-103, 443 (1999).



K. Ueda et al., Phys. Rev. A 54, 490 (1996).

Conclusion

Base-molecule-specific electronic structures near the Fermi level of DNA

- **Excited electrons into the π* state affect the Auger transitions**
- **Finite lifetime (≥ 10^{-14} s) of the π* state electrons**
- **Electrons in the π* state are localized.**

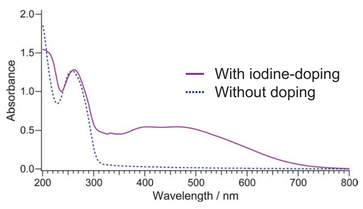
→ **Charge Hopping for Conduction (Model 2)**

H.S. Kato, M. Furukawa, M. Kawai, M. Taniguchi, T. Kawai, T. Hatsui, and N. Kosugi, Phys. Rev. Lett. **93** (2004) 086403

Characterization of Iodine-doped DNA

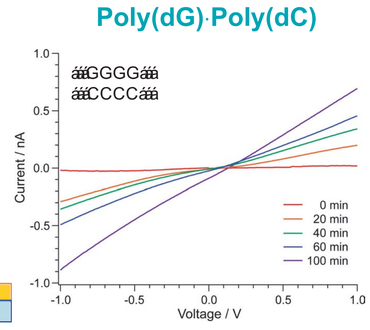
共同研究：　分子研　初井宇記、小杉信博
阪大産研　谷口正輝、川合知二
広大　吉田智喜、相田美砂子

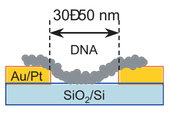
Introduction



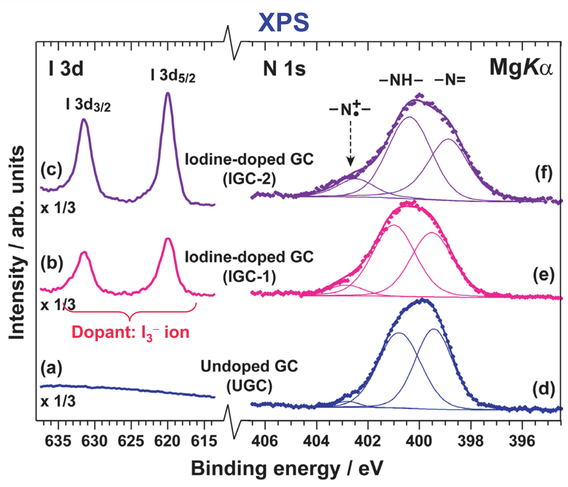
M. Taniguchi et al., JJAP 42 (2003) L215

Poly(dG)·Poly(dC)

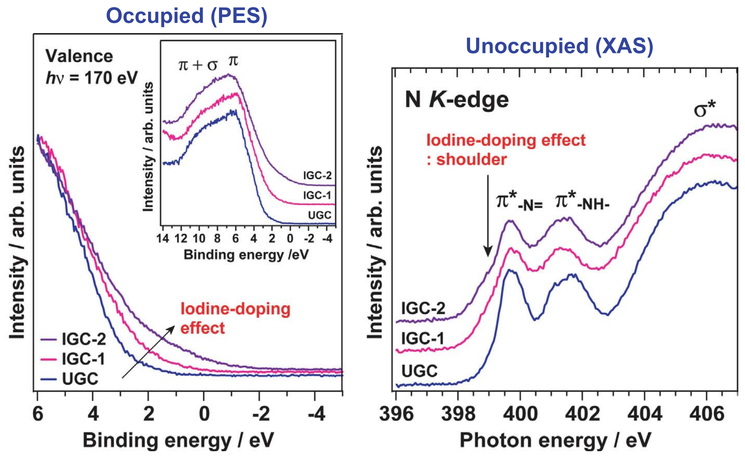




Photoemission & X-ray Absorption

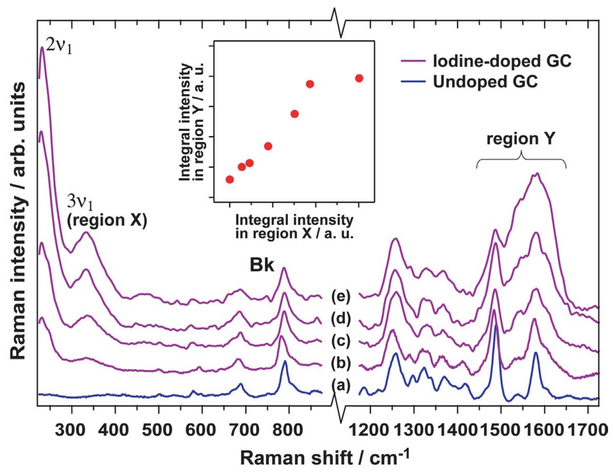


Radical cation formation in DNA bases

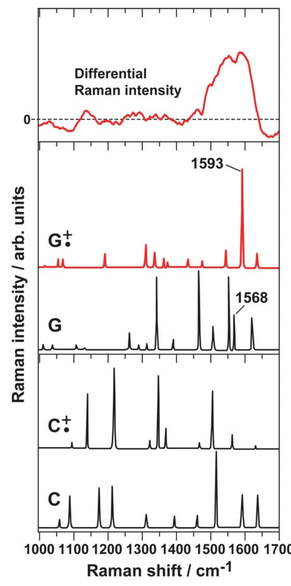


New electronic states in the intrinsic band gap

Raman Spectroscopy & DFT calculations

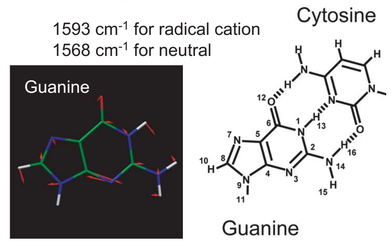


$2\nu_1$, $3\nu_1$: 2nd- and 3rd-harmonics of stretch vibration of I_3^-
Bk: Stretch vibration of O-P-O in the backbone



DFT calculation

1593 cm^{-1} for radical cation
1568 cm^{-1} for neutral



Radical cation formation at **Guanine** *site*

Conclusion

Elucidation of conductivity enhancement at iodine-doped DNA

- **Radical cation formation at Guanine bases**
- **Appearance of new electronic states in the intrinsic band gap**

→ **Formation of the Small Polaron**
(Characteristics of conductive polymers)

M. Furukawa, H.S. Kato, M. Taniguchi, T. Kawai, T. Hatsui, N. Kosugi, T. Yoshida, M. Aida and M. Kawai, Phys. Rev. B **75** (2007) 045119