2nd LATAM MEETING ON GREEN AMMONIA AND POWER-to-X

MatER Materials Science and Renewable Energies Group

Aluminum-Doped Amorphous Silicon Carbide Thin Films as Photocathode for Green Ammonia Production

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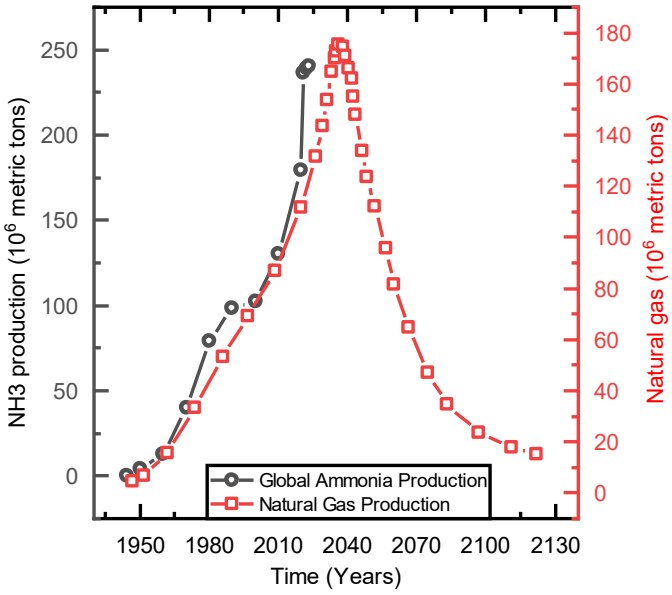
CAMPUCP CENTRO DE CARACTERIZACIÓN DE MATERIALES

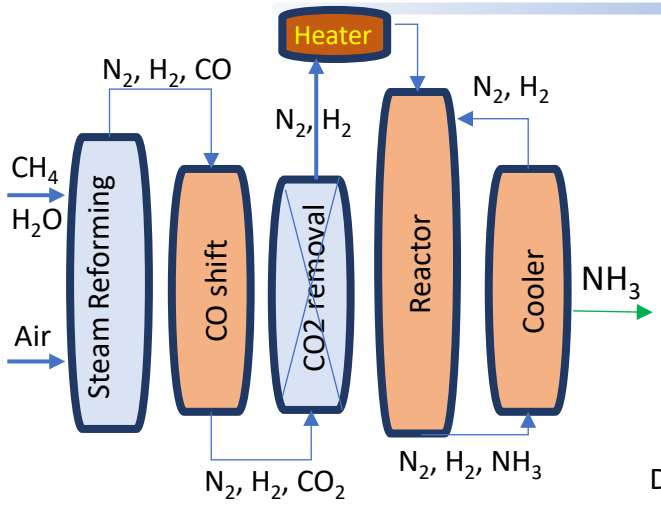
CONCYTEC CONSEJO NACIONAL DE CIENCIA, TECNOLOGÍA E INNOVACIÓN

ProCIENCIA

Introduction



Palma, V. et al. Nanomaterials,(2020),1-56,10(8)



$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(l)}$$

Palma, V. et al. Nanomaterials,(2020),1-56,10(8)

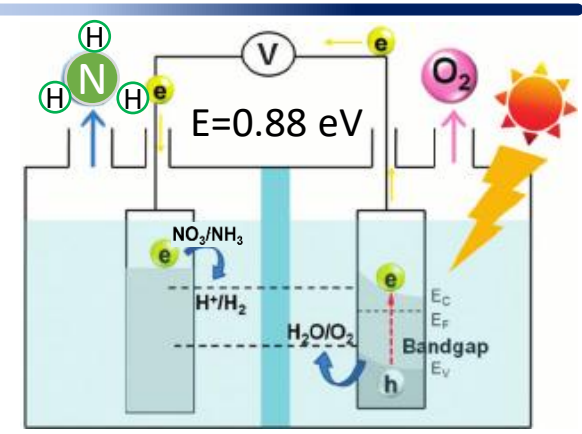
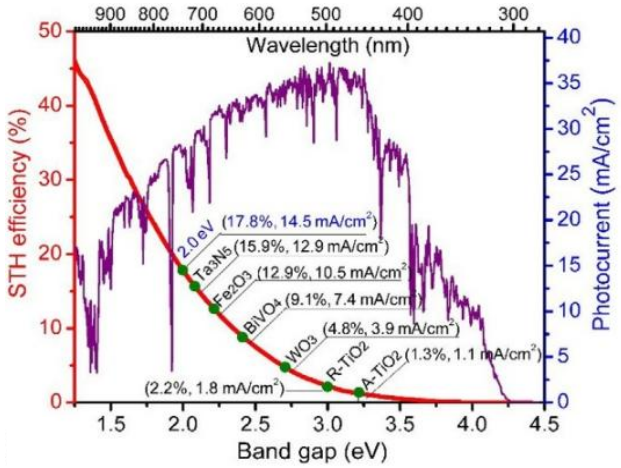


Diagram of the basic principles of Reduction NO_3 for photoelectrochemical cell

Chen, H. et al. Chemical Society Review,(2012),5654-5671,41(17)



Jian et al. Solar RRL, 2020,4(7)

Why a-SiC?

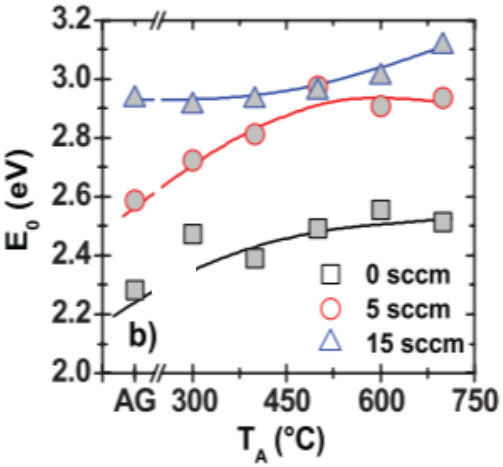
- ❑ Abundance and easy reproducible
- ❑ Band gap tunning
- ❑ Excellent chemical stability

Soltys et al. Physics and chemist of solid state(2023),5-16,24(1)

What we aim?

- ❑ Physical properties
- ❑ Photoelectrochemical properties

a-$Si_{1-x}C_x$



.Guerra et al.JournalPhysics,2016,49(19)

Potential and Electrochemical Response Analysis

$$W.E:\ NO_3^- + 9H^+ + 8e^- + hv \rightarrow NH_4^+ + 3H_2O\ \left(E^0_{red} = +0.88\,V\right)$$

$$C.E:\ H_2O \rightarrow 4H^+ + O_2 + 4e^-\ \left(E^0_{red} = -1.23\,V\right)$$

Karamad et al.2022

Cathode	Overpotential (η vs Ag/AgCl)	
Pt	-0.3 a -0.8 V	Zhang H. et al 2023
RuCo	-0.4 a -0.9 V	Hang et al.2023
CuO	-0.3 a -0.6 V	Bai L. et al.2021
SiC	-0.6 a -1.2 V	Guo W. et al.2023

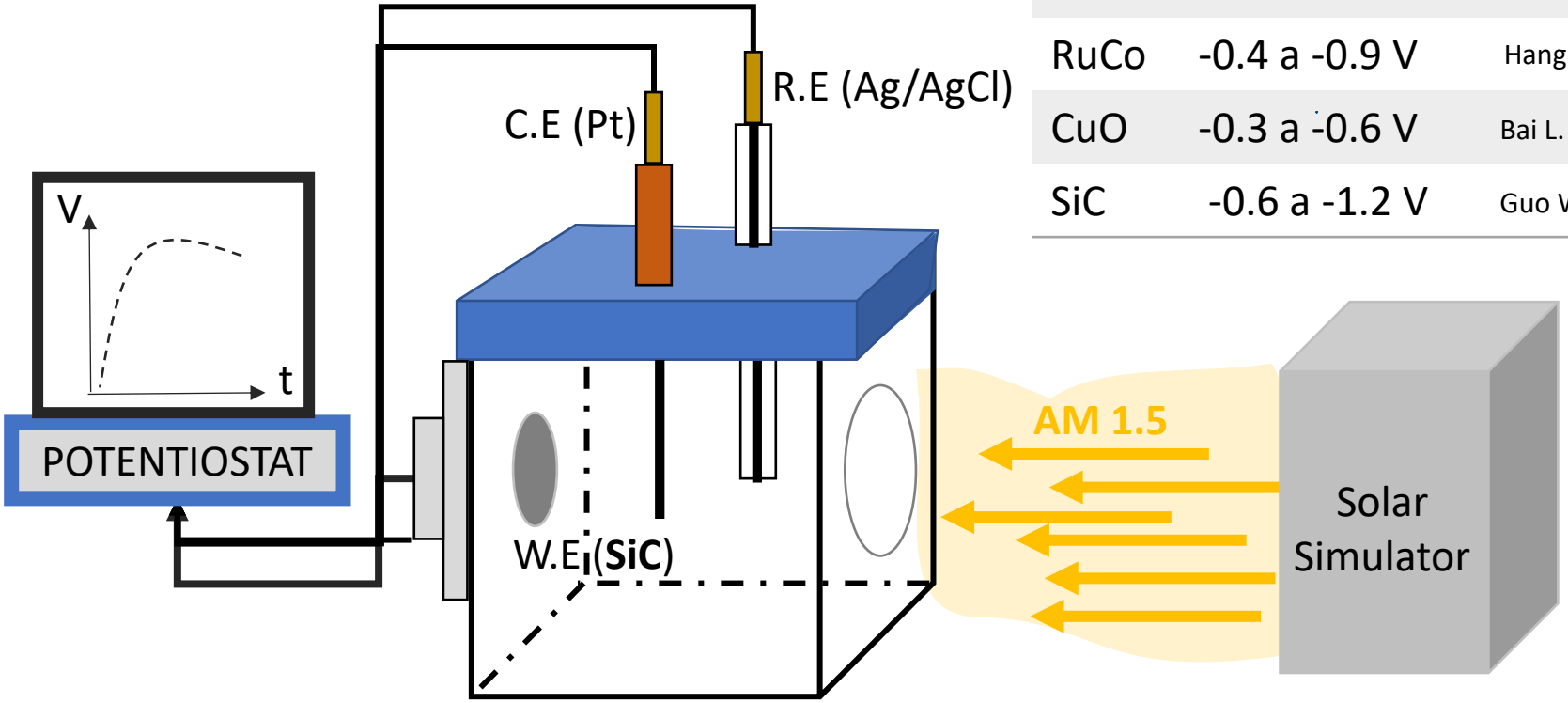
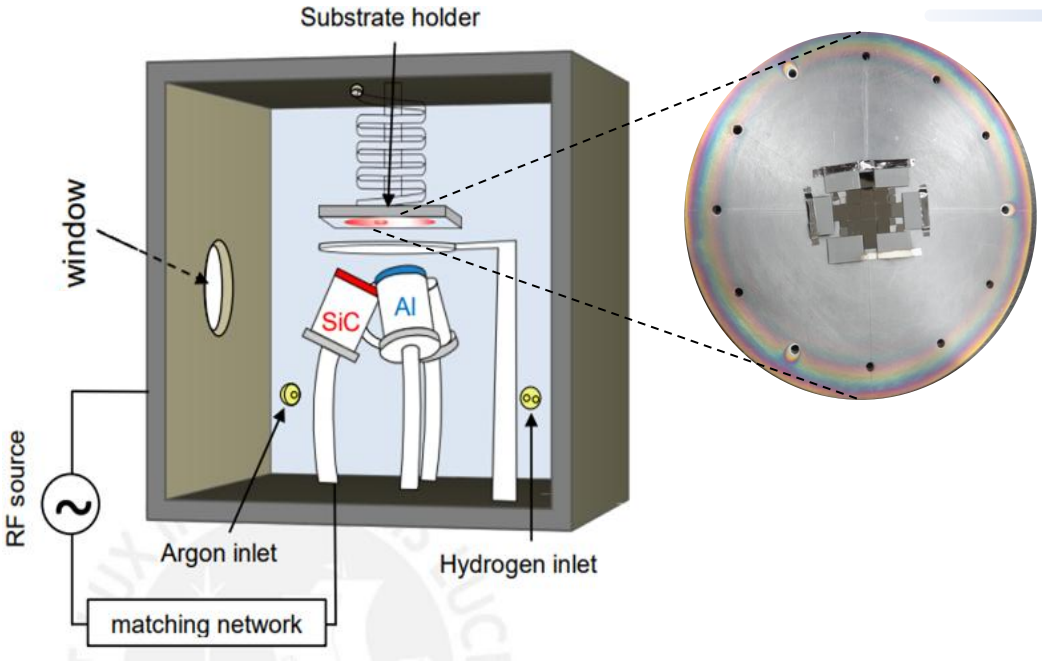


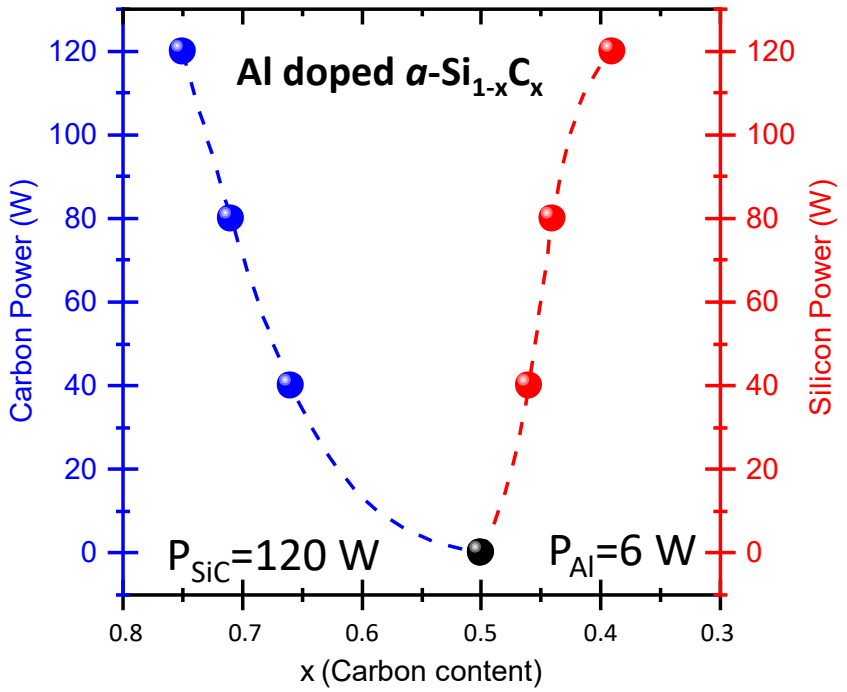
Diagram for evaluation photoelectrochemical response

Thin Film Deposition



Magnetron Sputtering arrangement

$$R_{SiC} = 0.045P_{SiC} - 0.53$$

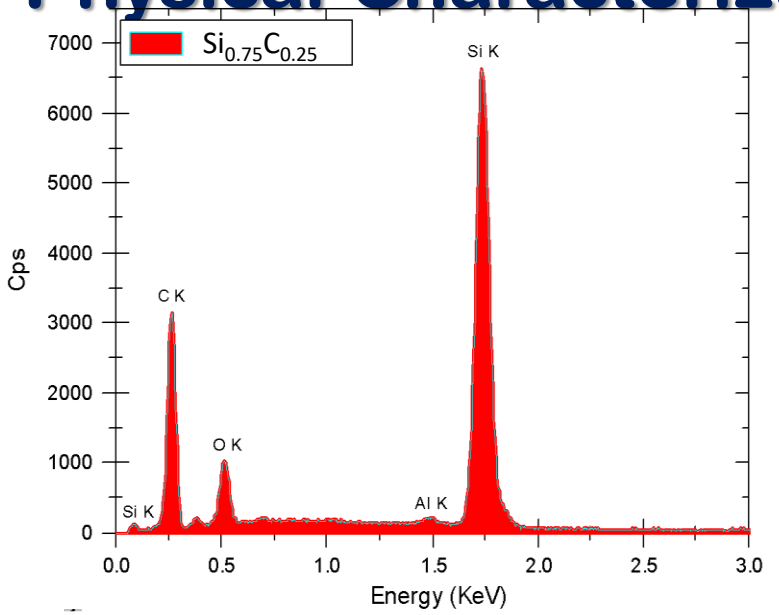


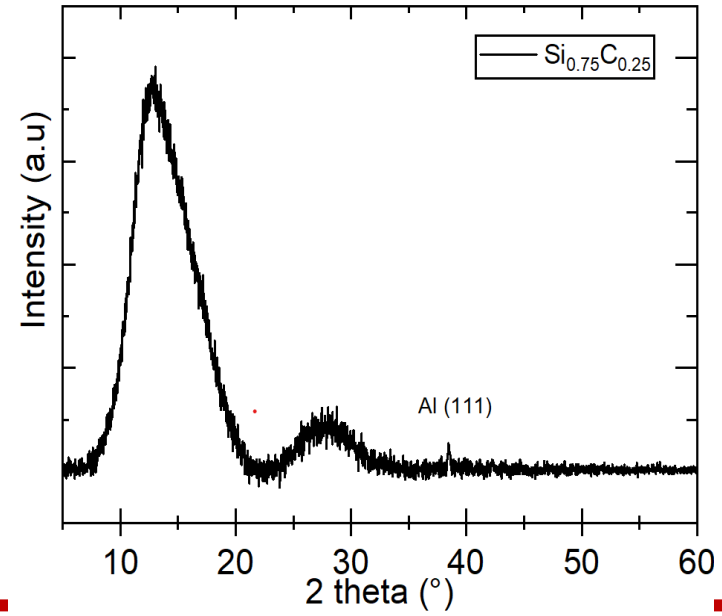
Plot of targets power to get *a*-$Si_{1-x}C_x$:Al thin films

- Base Pressure: $3.5 \times 10^{-7} mbar$.
- Active cooling and rotation of substrate holder at 10 °C
- Argon flux of 30 sccm
- Deposition time : 45 min.

Images of sputtered of non-stoichiometric *a*-$Si_{1-x}C_x$:Al thin films

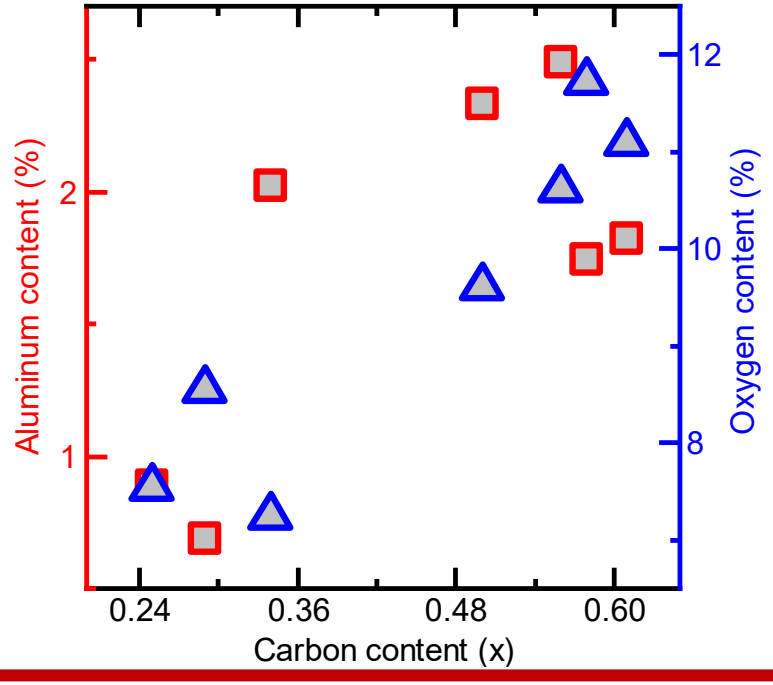
Physical Characterization



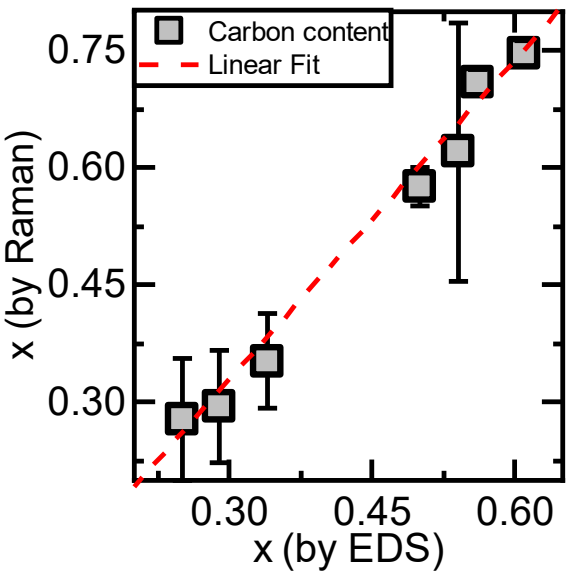


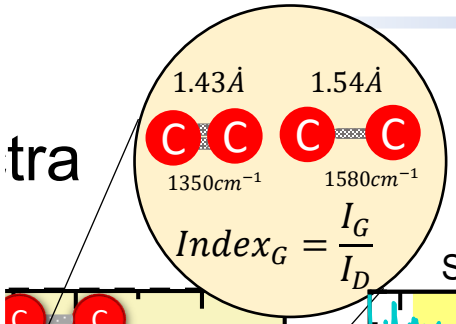
	Chemical composition (Atomic %)			
	Si	C	O	Al
$Si_{0.75}C_{0.25}$	66.51	**25.06**	7.54	0.89
$Si_{0.75}C_{0.29}$	61.85	**28.91**	8.55	0.69
$Si_{0.64}C_{0.34}$	57.16	**33.07**	7.24	2.02
$Si_{0.50}C_{0.50}$	41.11	**46.95**	9.60	2.33
$Si_{0.44}C_{0.56}$	34.99	**51.90**	10.62	2.49
$Si_{0.42}C_{0.58}$	33.35	**53.15**	11.73	1.74
$Si_{0.39}C_{0.61}$	30.38	**54.91**	11.10	1.82

Elemental atomic concentration of samples produced by RF magnetron sputtering.



Structure and bonding of a-SiC





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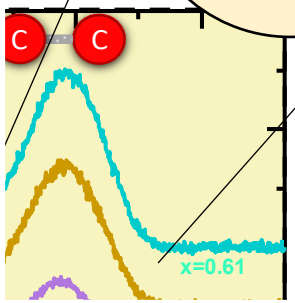
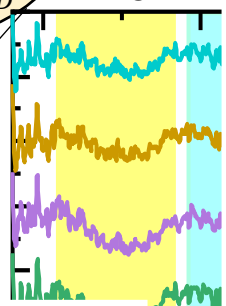
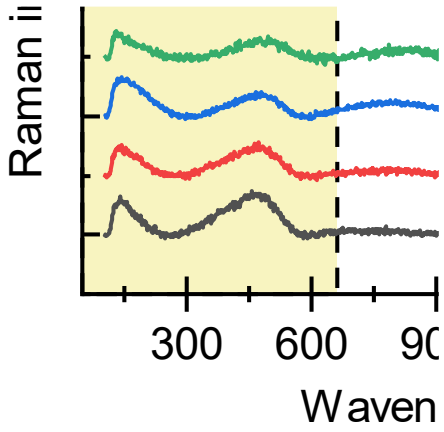
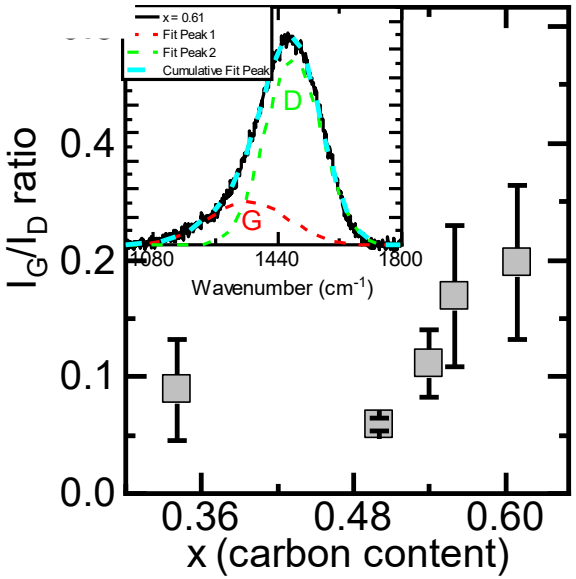
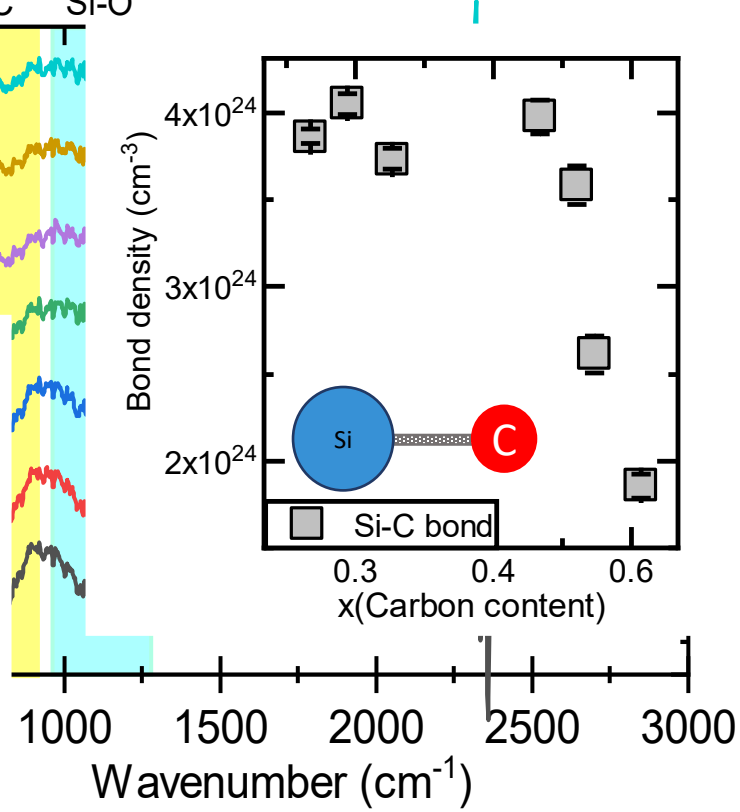




IR Spectra

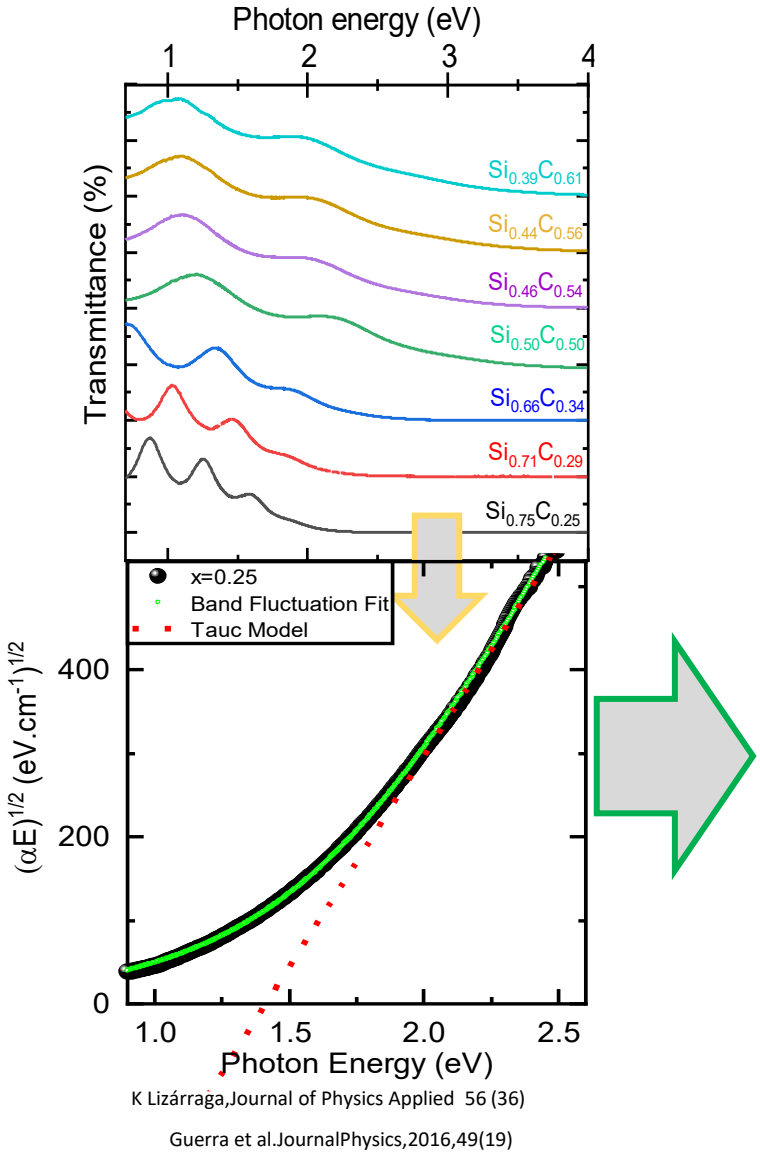






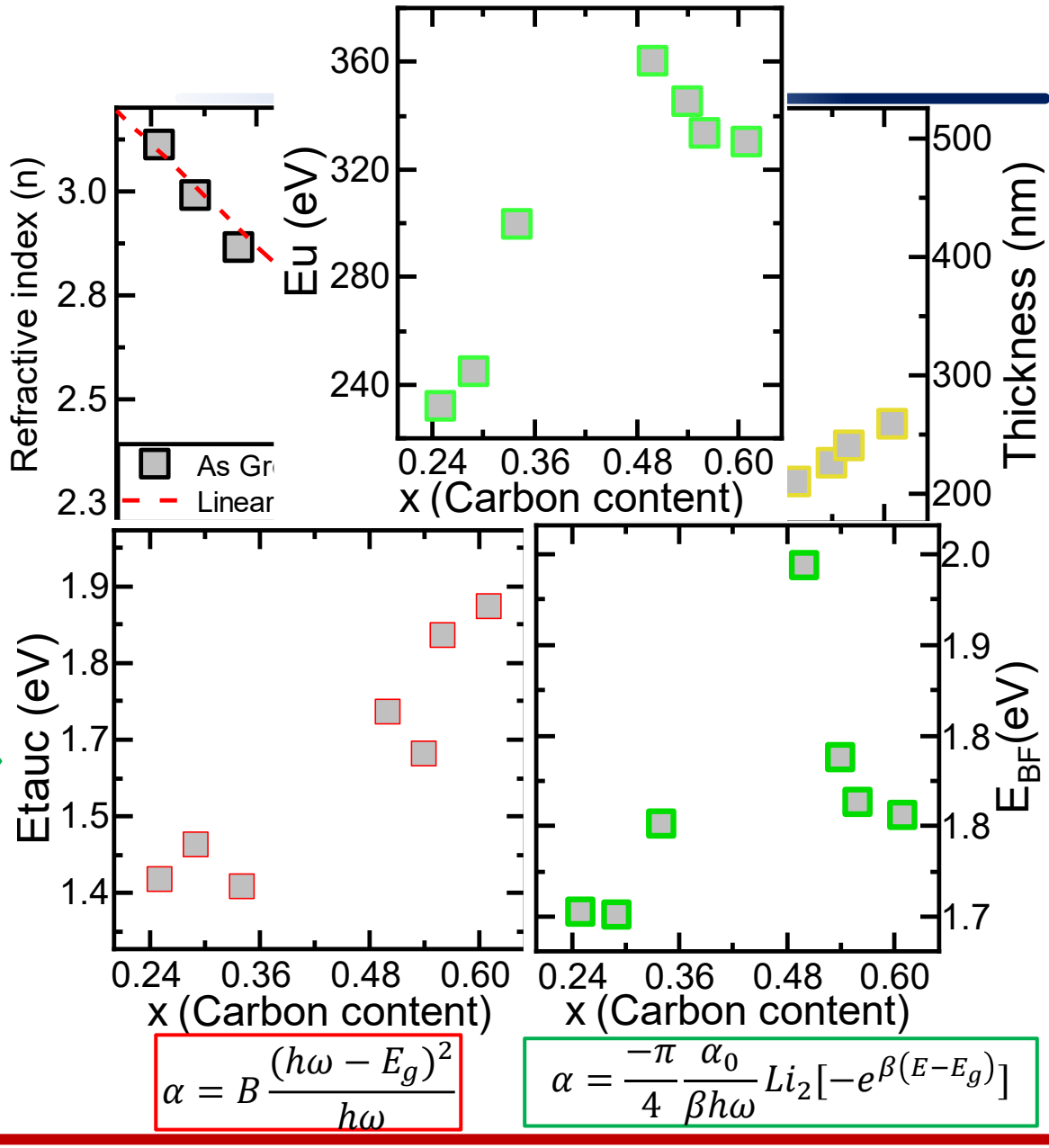
Gallis S. et Journal of Applied Physicsal.2007,102(2)

Optical characterization



K Lizárraga,Journal of Physics Applied 56 (36)

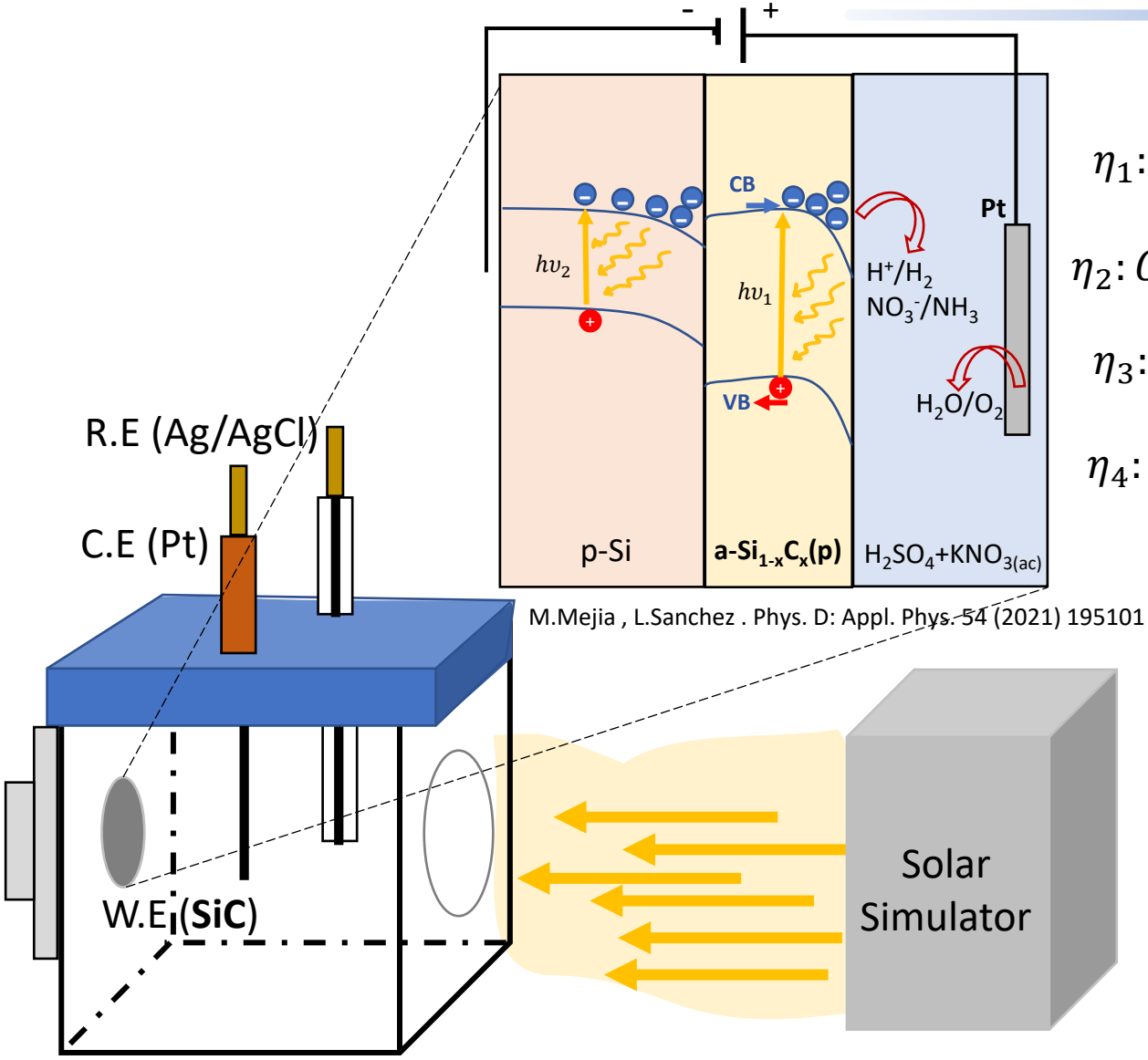
Guerra et al.JournalPhysics,2016,49(19)



$$\alpha = B\frac{(h\omega - E_g)^2}{h\omega}$$

$$\alpha = \frac{-\pi}{4}\frac{\alpha_0}{\beta h\omega}Li_2[-e^{\beta(E-E_g)}]$$

Photoelectrochemical characterization



M.Mejia , L.Sanchez . Phys. D: Appl. Phys. 54 (2021) 195101

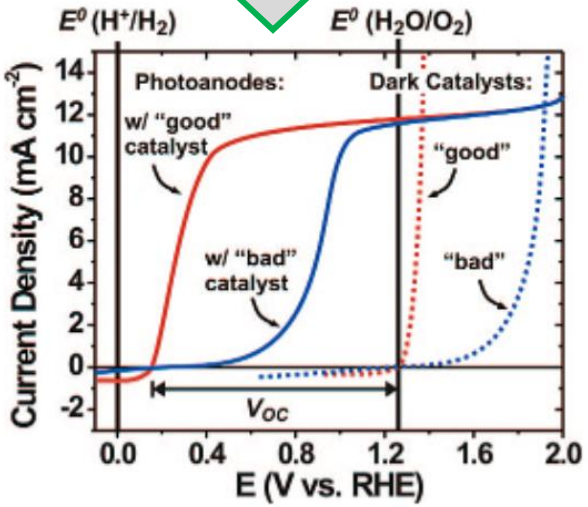
$$\eta_{PEC} = \eta_1 . \eta_2 . \eta_3 . \eta_4$$

η_1: *Light harvesting efficiency*

η_2: *Charge separation efficiency*

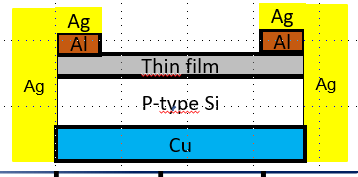
η_3: *Charge transport efficiency*

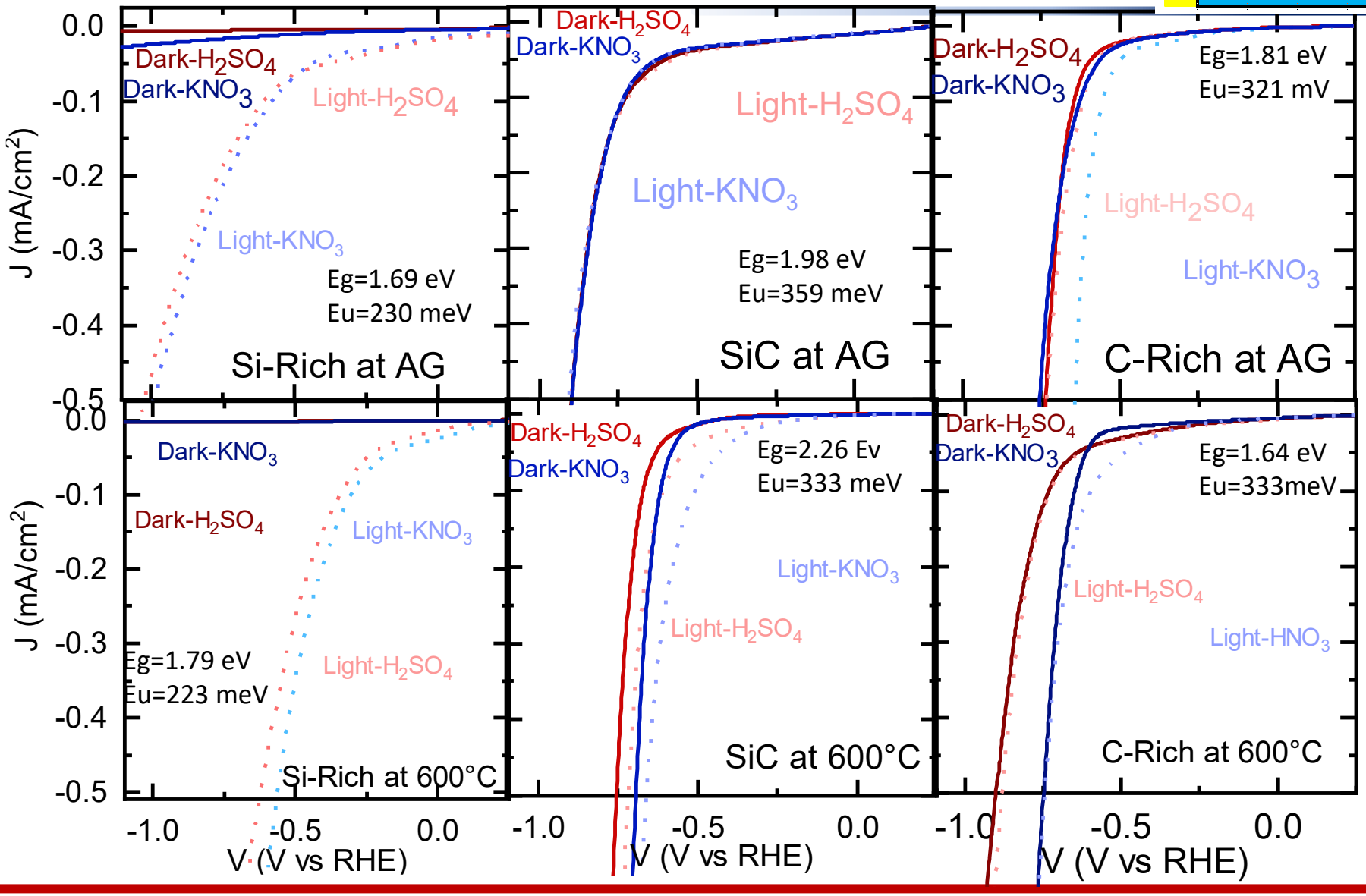
η_4: *Surface reaction efficiency*



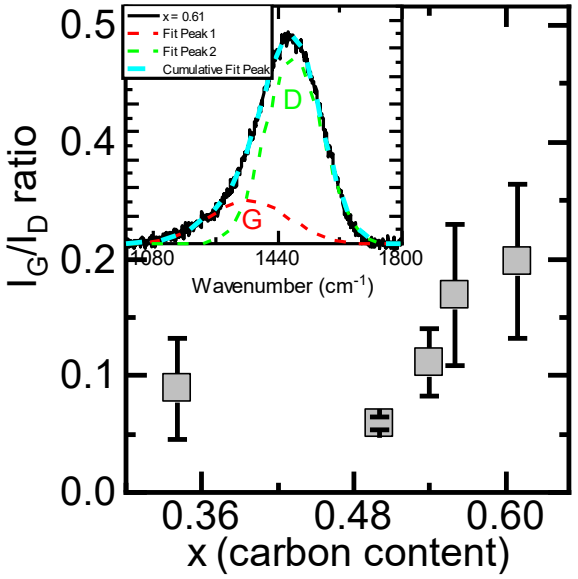
Michael G. Chem.Rev.2010,110,6446-6473

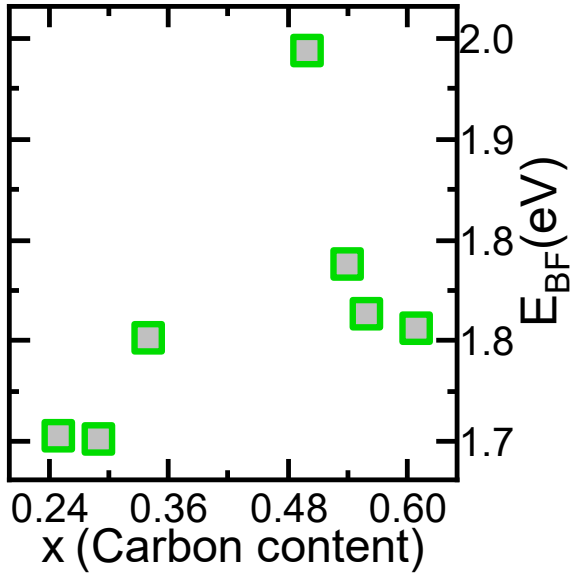
Photoelectrochemical characterization

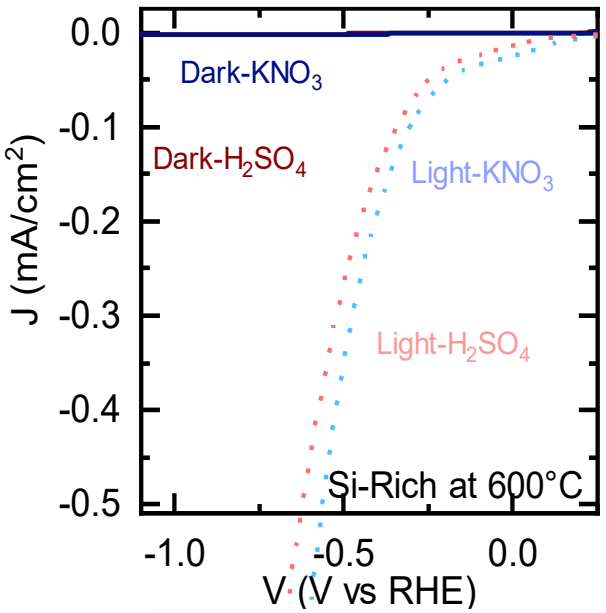




Summary and future work







- Do electrolytes of SiC substochiometric at 600°C and quantify the ammonia production.
- Determine flat band potential and dopants through Mott-Schottky plots of SiC substochiometric samples
- Do electrolytes of cocatalysis loading of silicon rich sample at AG and quantify the ammonia production.

Acknowledgements

Prof. Dr. Andrés Guerra
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Prof. Dr. Kamala Nanda
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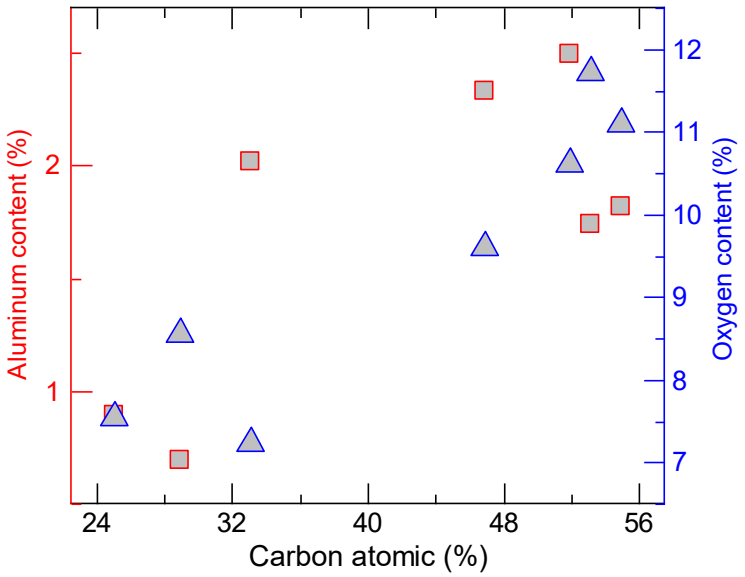
THANKS

EDS measurement



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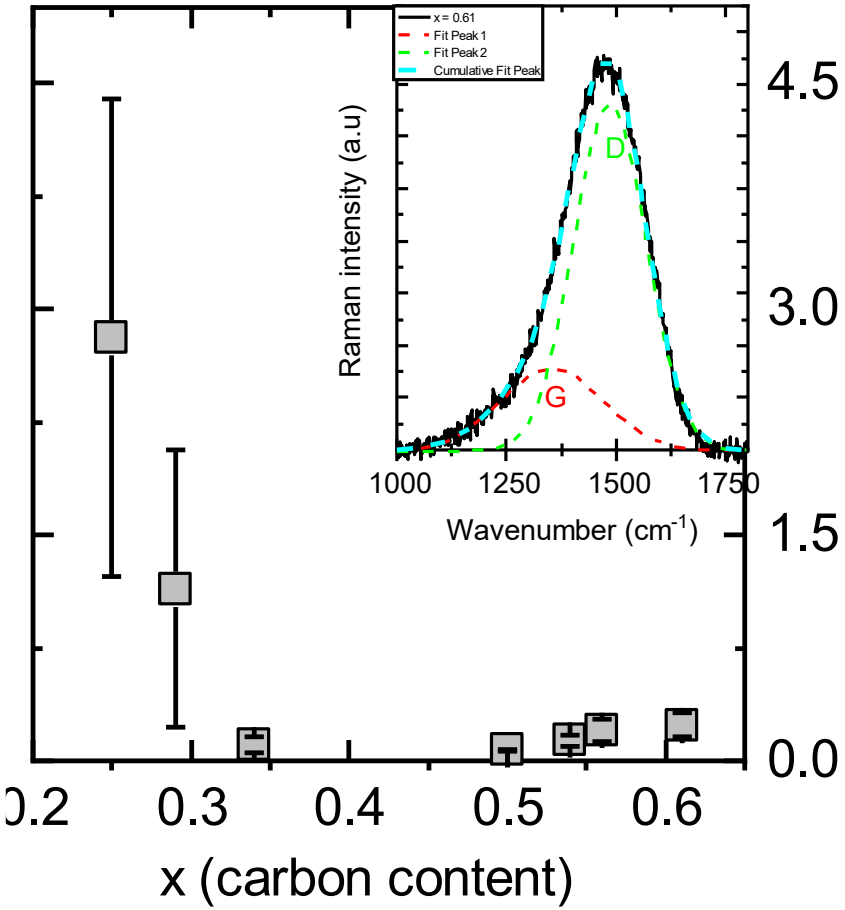
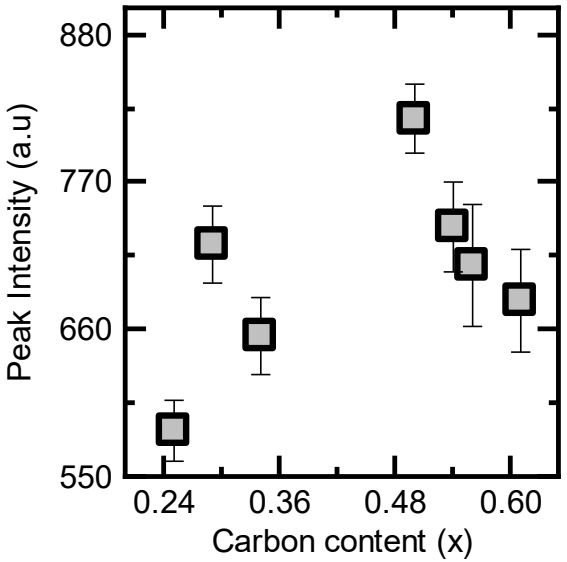
Index Graphitization





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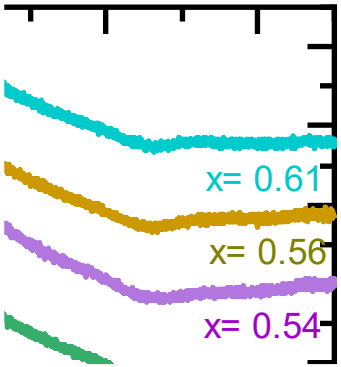
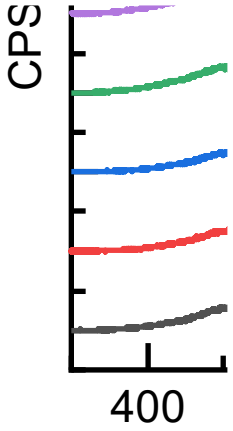
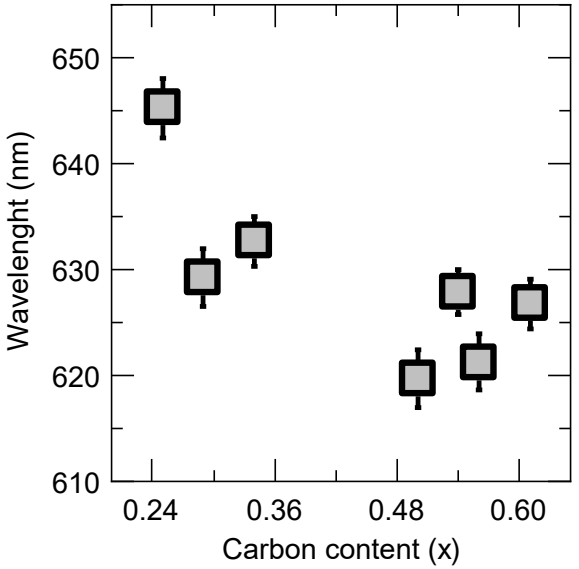
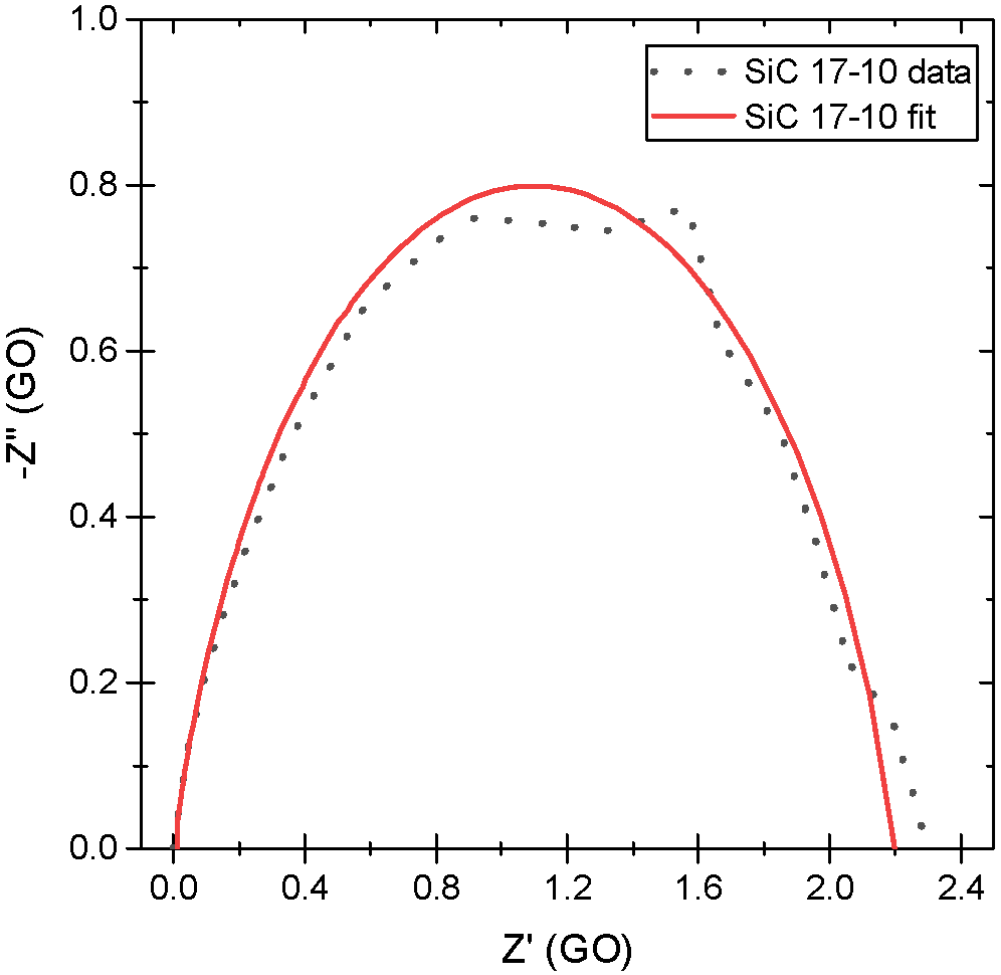


I_G/I_D



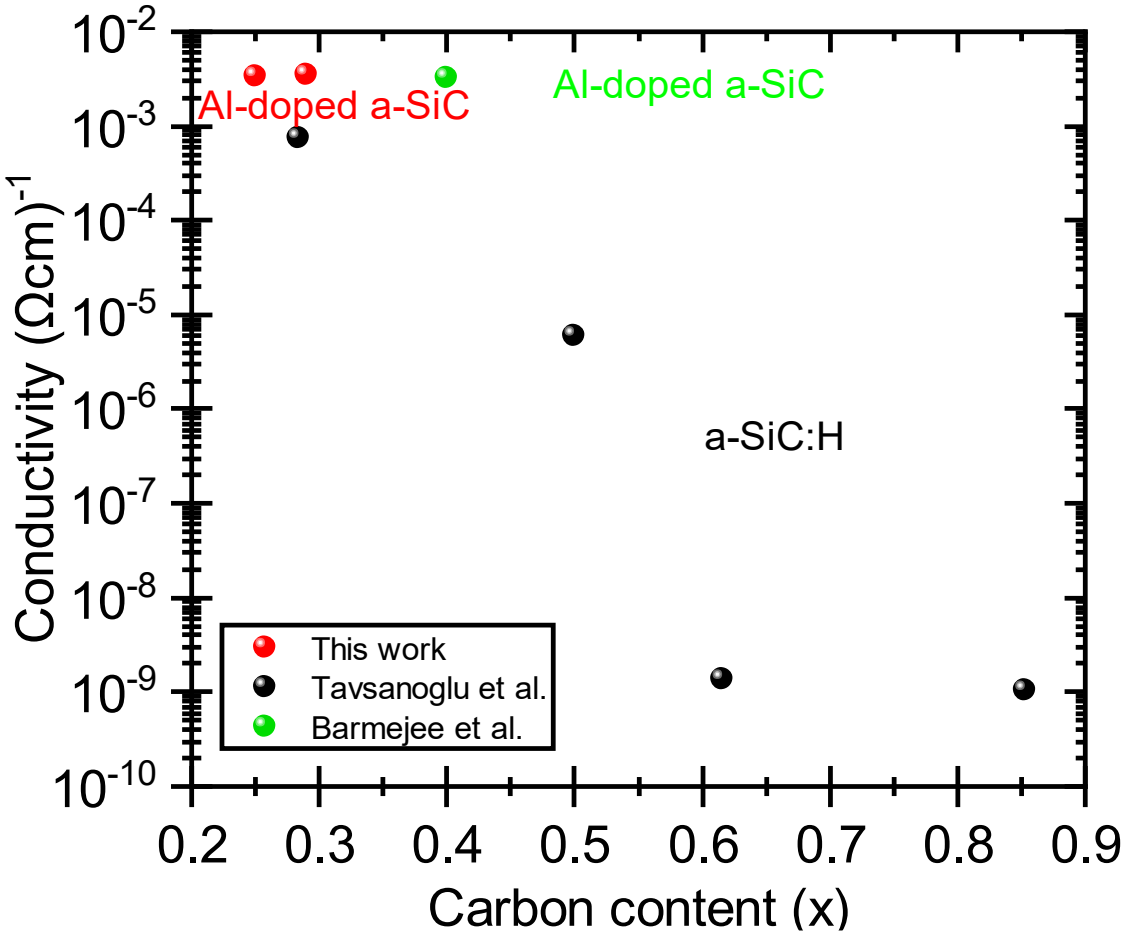


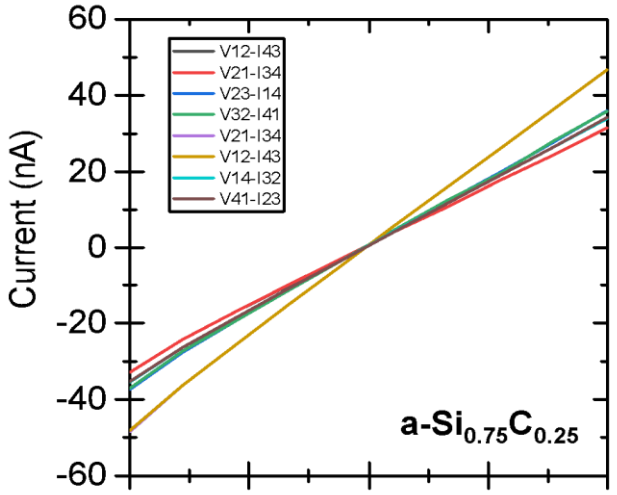
EIS semiconductor



Parameters (Unit)	Value
Bulk resistance (GΩ)	2.2
CPE (pF)	0.54
Equivalent Capacitance (pF)	0.10
index	0.80
Maximum frequency (Hz)	713
Conductivity (S/m)	0.455x10-9
Relative permittivity	14

Electrical measurement

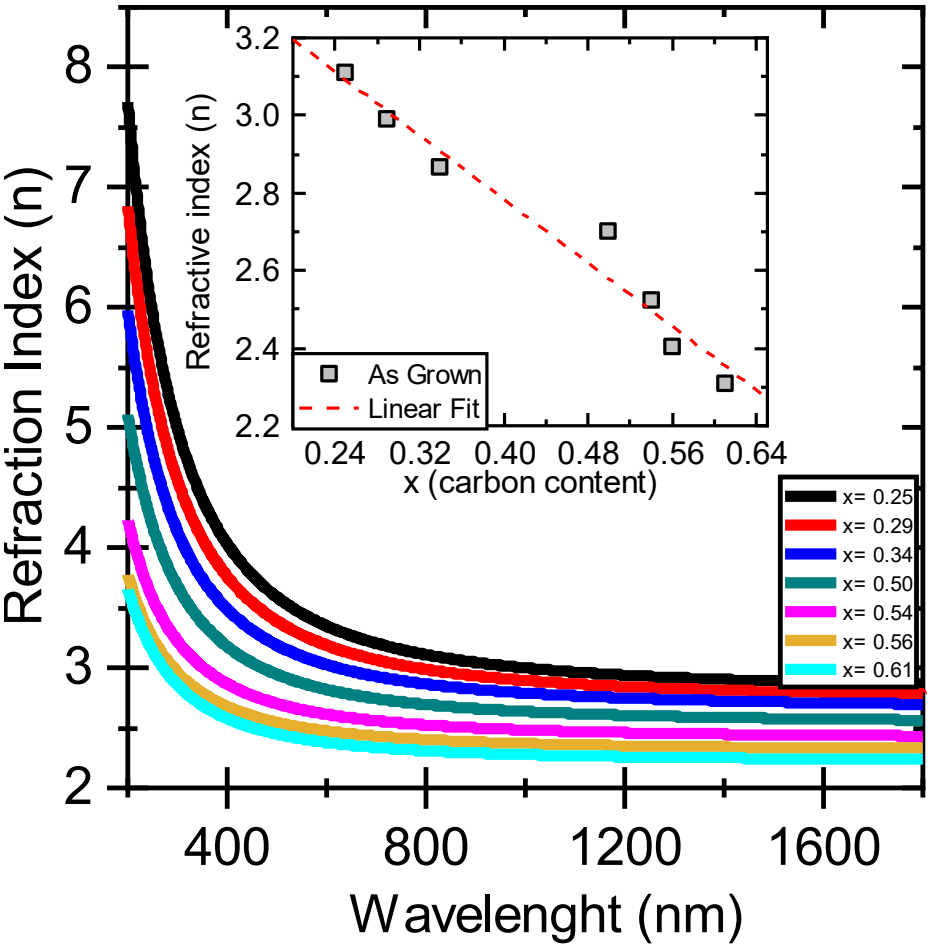


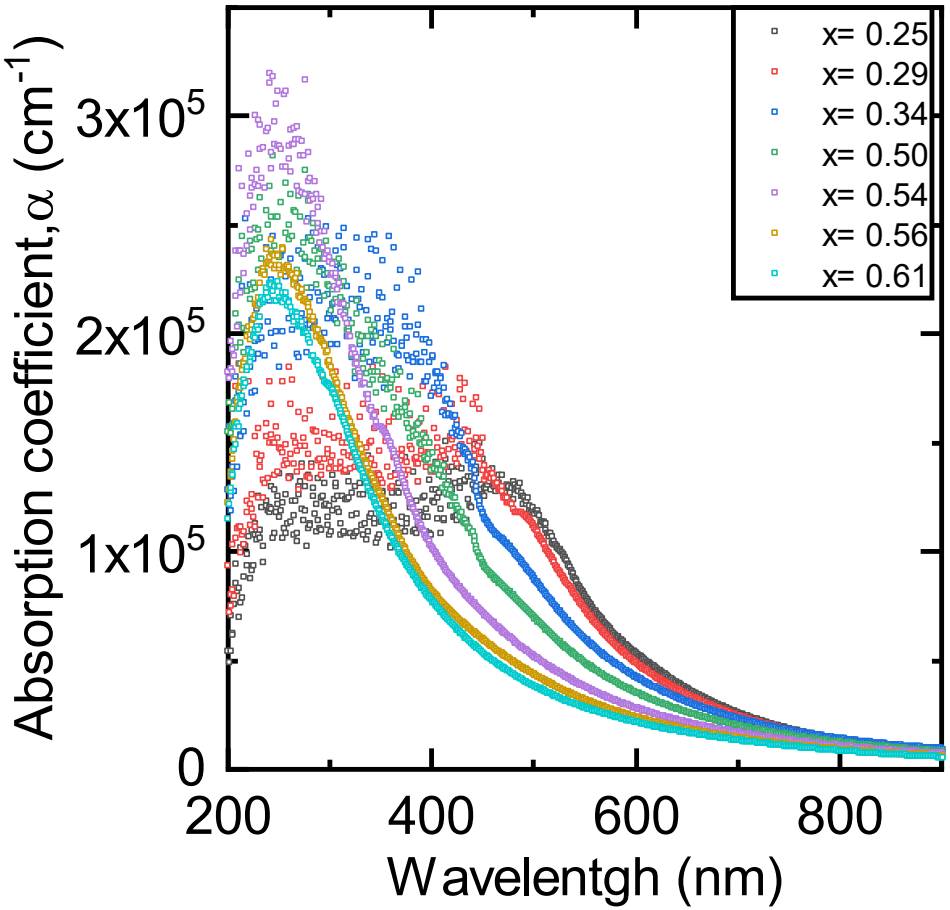


Samples	Conductivity (Ω^{-1} cm^{-1})
σ (x=0.25)	3.53 x10^{-3}
σ (x=0.29)	3.45x10^{-3}
σ (x=0.34)	—------
σ (x=0.50)	-------
σ (x=0.56)	----------
σ (x =0.58)	----------
σ (x=0.61)	--------

Conductivity values of SiC films [8][9]

Optical measurement





EIS measurement