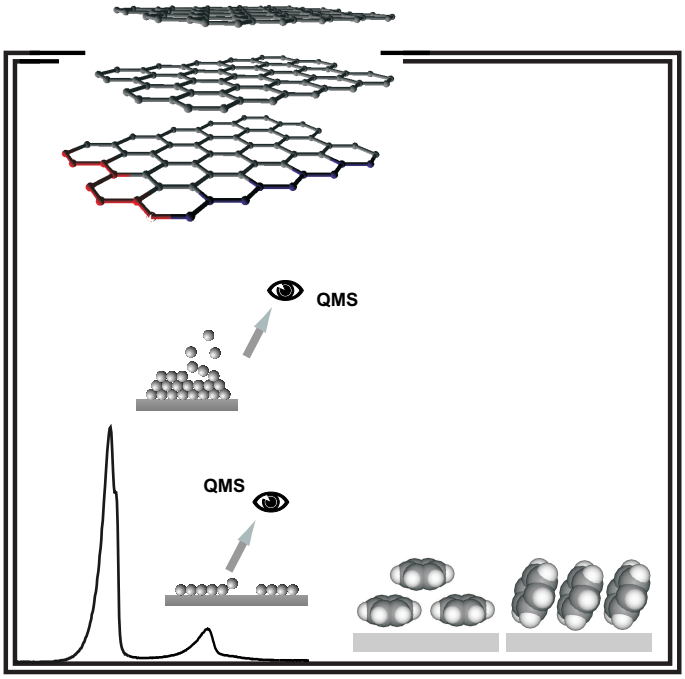
Desorption of gases from graphitic and porous carbon surfaces



Dissertation

zur Erlangung des akademischen Grades

doctor rerum naturalium

im Fachbereich Chemie der Freien Universität Berlin
eingereichte Dissertation

von

M.Sc. Renju Zacharia
aus Kottayam, Indien

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May 2004
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Gutachter

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2. Prof. Dr. R. Schlögl

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Abbrevations and acronyms

CDD	*Coupled desorption diffusion*
CNF	*Carbon nanofiber*
CNT	*Carbon nanotube*
DFT	*Density functional theory*
ER	*Eley-Rideal Mechanism*
FM	*Falconer-Madix method*
HOPG	*Highly oriented pyrolytic graphite*
LH	*Langmuir-Hinshelwood mechanism*
LEED	*Low energy electron diffraction*
MvK	*Mars-van Krevelen mechanism*
MM3	*Molecular mechanics force field 3*
MWNT	*Multi-wall carbon nanotube*
ML	*Monolayer*
ODH	*Oxidative dehydrogenation*
PAH	*Polyaromatic hydrocarbon*
QMS	*Quadrupole mass spectrometer*
STM	*Scanning tunnelling microscopy*
SWNT	*Single-wall carbon nanotube*
TEM	*Transmission electron microscopy*
TD	*Thermal desorption*
TDS	*Thermal desorption spectroscopy*
TPD	*Temperature programmed desorption*
TST	*Transition state theory*
UHV	*Ultrahigh vacuum*
vdW	*van der Waals*

List of Symbols

α	*molecular static polarizability*	Å^3
α_{zz}	*z-component of polarizability tensor*	Å^3
β	*heating rate*	$\text{K}\,\text{s}^{-1}$
ν	*frequency factor*	s^{-1}
σ	*number of adsorbates per unit area*	m^{-2}
θ	*surface coverage*	ML
$[A]_g$	*gas phase concentration of adsorbate A*	$\text{mol}\,\text{m}^{-3}$
$[A]_s$	*surface concentration of adsorbate A*	$\text{mol}\,\text{m}^{-2}$
C_{EB}	*percentage conversion of ethylbenzene*	-
E_b	*binding energy*	eV
E_{cl}	*cleavage energy of graphite*	eV
E_d	*activation energy of desorption*	eV
k_i	*rate constant*	$\text{mol}\,\text{m}^{-3}\,\text{s}^{-1}$
k_B	*Boltzmann constant*	$\text{J}\,\text{K}^{-1}$
m	*molecular mass*	kg
n	*order of desorption*	-
s, s_0	*sticking coefficient*	-
S_{ST}	*selectivity to form styrene*	-
T, T_0, T_{max}	*temperature*	K
p, p_0	*pressure*	mbar
V_{vdW}	*van der Waals potential*	eV