Characterization of fundamental catalytic properties of MoS_2/WS_2 nanotubes and nanoclusters for desulfurization catalysis – a surface chemistry study

DoE final report

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List of acronyms and abbreviations

AFM	atomic force microscopy
CMA	cylindrical mirror analyzer
CNTs	carbon nanotubes
CVD	chemical vapor deposition
DFT	density functional theory
EBL	electron beam lithography
EDX/EDS	energy dispersive X-ray spectroscopy
GC	gas chromatograph
HDS	hydrodesulfurization
HREELS	high resolution electron energy loss spectroscopy
IF	inorganic fullerene-like nanoparticles
LEED	low energy electron diffraction
MCS	Monte Carlo simulations
NDSU	North Dakota State University
NT	nanotubes
NP	nanoparticles
PNNL	Pacific Northwest National Laboratory
PVD	physical vapor deposition
SEM	scanning electron microscopy
STM	scanning tunneling microscopy
TEM	transmission electron microscopy
TiNTs	TiO_2 nanotubes
TDS	thermal desorption spectroscopy
TOF	time of flight spectroscopy
UHV	ultra-high vacuum
UPS	ultraviolet photoelectron spectroscopy
UV	ultraviolet
XPS	x-ray photoelectron spectroscopy

Title of prior proposal "Characterization of fundamental catalytic properties of MoS$_2$/WS$_2$ nanotubes and nanoclusters for desulfurization catalysis – a surface chemistry study" **Prior DOE grant number:** DE-FG02-08ER15987
Duration of prior proposal 8/15/08 to 08/14/11   **Prior funding $352,000 (three years) + $65,000 (supplemental)**

1. Summary of projects (abstract) [1-18]

The prior project consisted of two main project lines. *First,* characterization of novel nanomaterials for hydrodesulfurization (HDS) applications. *Second,* studying more traditional model systems for HDS such as vapor-deposited silica-supported Mo and MoS$_x$ clusters.

In the first subproject, we studied WS$_2$ and MoS$_2$ fullerene-like nanoparticles as well as WS$_2$ nanotubes. Thiophene (C$_4$H$_4$S) was used as the probe molecule. Interestingly, metallic and sulfur-like adsorption sites could be identified on the silica-supported fullerene-particles system. Similar structures are seen for the traditional system (vapor-deposited clusters). Thus, this may be a kinetics fingerprint feature of modern HDS model systems. In addition, kinetics data allowed characterization of the different adsorption sites for thiophene on and *inside* WS$_2$ nanotube bundles. The latter is a unique feature of nanotubes that has not been reported before for any inorganic nanotube system; however, examples are known for carbon nanotubes, including prior work of the PI. Although HDS has been studied for decades, utilizing nanotubes as nanosized HDS reactors has never been tried before, as far as we know. This is of interest from a fundamental perspective. Unfortunately, the HDS activity of the nanocatalysts at ultra-high vacuum (UHV) conditions was close to the detection limit of our techniques. Therefore, we propose to run experiments at ambient pressure on related nanopowder samples as part of the renewal application utilizing a now-available GC (gas chromatograph) setup. In addition, Ni and Co doped nanocatalyts are proposed for study. These dopants will boost the catalytic activity.

In the *second* subproject of the prior grant, we studied HDS-related chemistry on more traditional supported cluster catalysts. Mo clusters supported by physical vapor deposition (PVD) on silica have been characterized. Two reaction pathways are evident when adsorbing thiophene on Mo and MoS$_x$ clusters: molecular adsorption and dissociation. PVD Mo clusters turned out to be very reactive toward thiophene bond activation. Sulfur and carbon residuals form, which poison the catalyst and sulfide the Mo clusters. Sulfided silica-supported MoS$_x$ samples are not reactive toward thiophene bond activation. In addition to S and C deposits, H$_2$, H$_2$S, and small organic molecules were detected in the gas phase. Catalyst reactivation procedures, including O$_2$ and atomic hydrogen treatments, have been tested. Cluster size effects have been seen: thiophene adsorbs molecularly with larger binding energies on smaller clusters. However, larger clusters have smaller activation energy for C$_4$H$_4$S bond activation than smaller clusters. The latter is consistent with early catalysis studies. Kinetics and dynamics parameters have been determined quantitatively.

We spent a significant amount of time on upgrades of our equipment. A 2nd-hand refurbished X-ray photoelectron spectrometer (XPS) has been integrated into the existing molecular beam scattering system and is already operational (supported by the DoE supplemental grant available in October 2009). We also added a time of flight (TOF) system to the beam scattering apparatus and improved on the accessible impact energy range (new nozzle heater and gas mixing manifold) for the beam scattering experiments. In addition, a GC-based powder atmospheric flow reactor for studies on powder samples is now operational. Furthermore, a 2nd UHV kinetics system has been upgraded as well.

In summary, mostly single crystal systems have so far been considered in basic science studies about HDS. Industrial catalysts, however, can be better approximated with the supported cluster systems that we studied in this project. Furthermore, an entirely new class of HDS systems, namely fullerene-like particles and inorganic nanotubes, has been included. Studying new materials and systems has the potential to impact science and technology. The systems investigated are closely related to energy and environmental-related surface science/catalysis. This prior project, conducted at NDSU by a small team, resulted in a total of 14 printed publications,[1-5, 7-12, 14, 19, 20] eight months before the end of the funding period. In addition, collaborators at national laboratories and abroad were part of the projects, as proposed. More specifically, projects about HDS on MoS$_2$ and WS$_2$ inorganic fullerene-like nanoparticles,[1, 5] inorganic WS$_2$ nanotubes,[2] Mo and MoS$_2$ vapor-deposited nanoclusters,[3] modeling,[19] reviews/book chapter,[7, 11] and side projects[8-10] have been conducted, as proposed, acknowledging solely (exception ref.[7]) funding from this grant. A list of publications and coworkers is given in sect. 6.

2. Task 1 – Modern nanocatalysts as HDS (hydrodesulfurization) model systems

We studied HDS-related catalysis on WS_2 and MoS_2 fullerene-like nanoparticles and WS_2 nanotubes. The object was to evaluate if nano-sized novel materials show improved or different catalytic properties for HDS compared with the micro-sized catalysts used today in most industrial applications.

a) WS_2 *inorganic fullerene-like nanoparticles supported on silica as novel HDS catalysts*[5]

The reactive and non-reactive adsorption kinetics of thiophene (C_4H_4S) on WS_2 nanoparticles with fullerene-like (onion-like) structures (IF inorganic fullerenes) were studied under ultra-high vacuum (UHV) conditions. Sample temperature ramping techniques (adsorption kinetics) were applied. At low temperatures, thiophene adsorbs molecularly. At higher temperatures, the formation of H_2S and alkanes in a hydrogen/thiophene ambient is evident on fully sulfided as well as reduced and oxidized WS_2 nanoparticles (surface reactions).

Although some of the nanomaterials used in this project have become commercially available in bulk quantities, powders consisting of nanoparticles and nanotubes (see below) were provided by R. Tenne (Israel),

Fig. 1: Thiophene TDS data for MoS_2 fullerene-like nanoparticles supported on silica. Sulfur and Mo-like adsorption sites for thiophene could be identified. (D: condensation peak).

as specified in the original proposal. The nanoparticles/nanotubes (NP/NT) were deposited on silica using the drop-and-dry technique. The sample morphology was characterized with SEM/TEM (scanning electron microscopy/transmission electron microscopy) at PNNL (by B.W. Arey). Since the PNNL SEM facility is heavily targeted by a large number of groups, we went to Argonne National Laboratory for later projects (collaboration with L. Ming).

The following results have been obtained:

- In collaboration with PNNL, the morphology and chemical composition of IF-WS_2 were characterized using energy-dispersive X-ray spectroscopy (EDX) and scanning electron microscopy (SEM), both before and after UHV kinetics experiments. No significant changes in morphology or chemical composition were found.
- Thiophene adsorbed molecularly on pristine (fully sulfided) IF-WS_2 samples at low temperatures, as verified by multi-mass thermal desorption spectroscopy (TDS).
- Thiophene binding energies are in the range of 43–60 kJ/mol, depending on coverage.
- The HDS activity of pristine IF-WS_2 at UHV conditions was close to the detection limit of the mass spectrometer used. (This is in contrast to IF-MoS_2; see below.) Nevertheless, H_2S and alkane fragments were detected.
- Interestingly, partially reduced and oxidized samples are also catalytically active (toward HDS).
- The IF-WS_2 appears to be very stable.

b) MoS_2 *fullerene-like nanoparticles supported on silica*[1]

The catalytic activity of the rather new nanomaterial, IF-MoS_2 (inorganic fullerene-like nanoparticles), toward HDS activity has been characterized under UHV conditions. Thiophene TDS as well as quasi steady-state kinetics experiments have been conducted:
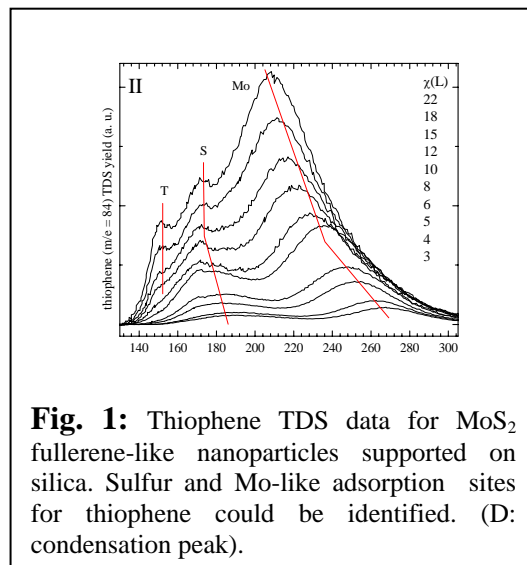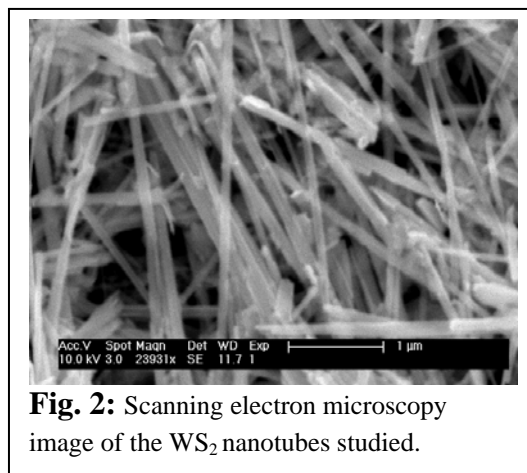
- Thiophene adsorbed molecularly on IF-MoS$_2$ at low adsorption temperatures. In addition to a condensation peak, two TDS features were observed, corresponding to binding energies of 46 and 52 kJ/mol (1 x 10^{13}/sec pre-exponential), respectively.
- Kinetics experiments with reduced and sulfided samples as well as spectroscopic data (Auger electron spectroscopy) suggest assigning the TDS peaks to sulfur- and Mo/MoO$_x$-like adsorption sites. Thus, we identified the active sites on the catalyst, which is a significant result (see Fig. 1), in our opinion.
- HDS activity was present in both the reduced and sulfided samples, but the largest HDS activity was seen in the reduced samples.

c) *WS$_2$ nanotubes supported on silica*[2]

Some problems with the preparation of the WS$_2$ nanotube samples for the surface chemistry experiments were initially encountered. Although the nanopowder samples consisted of 90% WS$_2$ nanotubes, as evident from the SEM images of the powders, the nanocatalyst supported by the drop-and-dry technique on silica was characterized by only debris and nanoparticles. Therefore, we collected the first data with solvent-free samples by pressing the powders in indium foil. Experimenting further with different solvents fortunately resulted finally in perfect WS$_2$ nanotube samples supported on silica (see Fig. 2). Solvent-free and drop-and-dry samples gave very similar results. The following data were collected on the supported WS$_2$ nanotubes.

Fig. 2: Scanning electron microscopy image of the WS$_2$ nanotubes studied.

- The adsorption kinetics of n-pentane, thiophene, and benzene on WS$_2$ nanotubes have been studied with TDS. Evidence has been obtained that these probe molecules adsorb on internal, external, and groove sites of the nanotubes bundles (see Fig. 3). Thus, different adsorption sites could be identified using a standard kinetics technique.
- Interestingly, for all probe molecules, distinct structures appeared in TDS data obtained for WS$_2$ NT that suggest, in an analogy to similar results obtained for carbon nanotubes (CNT) by our group[9, 14, 21] and others,[22] that TDS allows for distinguishing adsorption of the probe molecule on internal, external, and groove sites of the NT bundles. This is the first inorganic nanotube system reported in the literature where different adsorption sites could directly be identified. This is a quite exciting and pertinent result, in our opinion. Similar prior experiments with TiNTs, for example, failed due to their much smaller aspect ratio.[23, 24]
- Reactive TDS experiments at UHV conditions revealed some catalytic activity of the WS$_2$ NT toward HDS at amazingly low (200 K) reaction temperatures.
- Very few (basically none except our work) UHV studies have been performed on inorganic nanotubes as of 2010.[11, 14]

3. Task 2 – More traditional HDS model systems (vapor-deposited Mo and MoS$_x$ nanoclusters)[3]

The adsorption/decomposition kinetics/dynamics of thiophene have been studied on silica-supported Mo and MoS$_x$ clusters. Two-dimensional clusters form at small Mo exposures and large three-dimensional clusters at larger exposures, as characterized by Auger electron spectroscopy (AES). TDS indicates two reaction pathways. Thiophene desorbs molecularly at 190–500 K. Two different TDS features were evident and could be assigned to molecularly on Mo sites and sulfur (carbon) sites adsorbed thiophene. Assuming a standard pre-exponential factor for 1st-order kinetics, larger clusters are more reactive than smaller clusters for molecular adsorption of thiophene. The 2nd reaction pathway, the decomposition of thiophene, starts at 250 K. Utilizing multi-mass TDS, H$_2$, H$_2$S, and mostly alkanes are detected in the gas phase as decomposition products. The thiophene bond activation results in partially sulfided Mo clusters and carbon residuals on the surface, as characterized by AES. Sulfur and carbon poison the catalyst. As a result, as the number of thiophene adsorption/desorption cycles increases, the uptake of molecular thiophene decreases as well as the H$_2$ and H$_2$S production. Thus, at UHV conditions, sulfided silica-supported Mo clusters are less reactive than metallic clusters. The poisoned catalyst can be partially reactivated by annealing in oxygen. However, Mo oxides also appear

Fig. 3: Thiophene TDS on WS$_2$ nanotubes. In an analogy to the results on carbon nanotubes, the peaks have been assigned to different adsorption sites, namely internal (A), external (B), and groove sites (C) of thiophene on the inorganic nanotubes bundles. This is the first example of an inorganic nanotube in the literature where different adsorption sites could be identified. (D is the condensation peak.) Note that thiophene TDS of WS$_2$ fullerene-like nanoparticles consists of only one monolayer TDS structure. Similarly, support structures can be ruled out by conducting blind experiments on silica.

to form that passivate the catalyst further. On the other hand, when the used catalyst is annealed in hydrogen, the catalyst is poisoned even more, i.e., the sulfur AES signal increases. With adsorption transients (dynamics), the initial absorption probability, S$_0$, of thiophene has been determined. S$_0$ for molecular adsorption amounts to 0.43 ± 0.02 at 200 K and at thermal impact energies (E$_i$ = 0.04 eV). S$_0$ increases with Mo cluster size, obeying the capture zone model.[25, 26] The temperature dependence of S$_0$(T$_s$) consists of two regions consistent with molecular adsorption of thiophene at low temperatures and its decomposition above 250 K. Fitting S$_0$(T$_s$) curves allows one to determine the bond activation energy for the first elementary decomposition step of thiophene. Accordingly, larger clusters have smaller activation energies than smaller clusters.
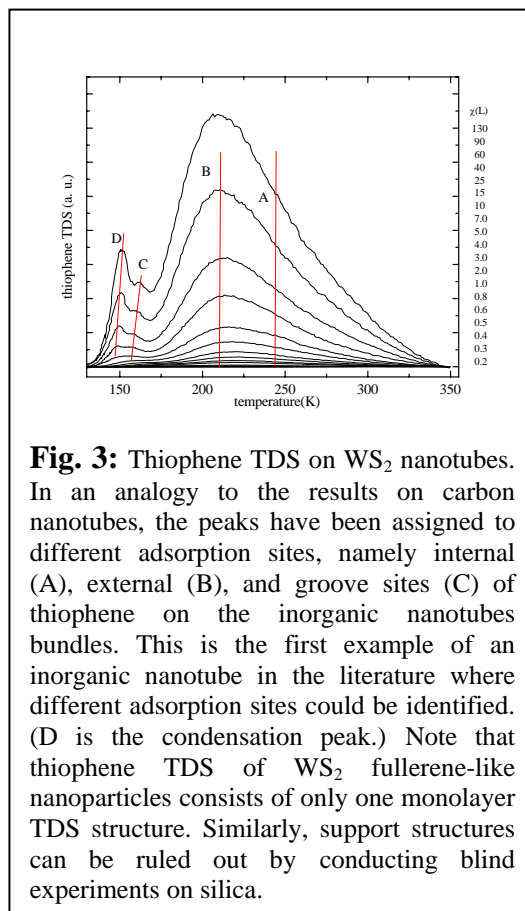
4. Task 3 – Modeling of kinetics data with time-resolved Monte Carlo simulations[6]

As we regularly use kinetics techniques such as TDS, it seems logical to work on a more sophisticated modeling of TDS data. As commercial software is unavailable, the PI's group has developed its own computer codes over the years.[27] In this subproject, a kinetic Monte Carlo simulation (KMCS) algorithm for simulating quantitatively experimental TDS data was developed. The KMCS is based on the master equation approach, and applies a first-passage time analysis, i.e., the time dependence of the kinetics is correctly matched. The KMCS-TDS scheme used here includes multiple kinetically distinct adsorption sites to model experimental data realistically. Furthermore, the effect of lateral interactions is included. This software can now readily be used to model new TDS data. Similar codes to model molecular beam scattering data are available in the PI's group.

5. Task 4 – Enlarging the experimental setup with an XPS (x-ray photoelectron spectroscopy) system (supplemental funding of prior project)

We have a second vacuum system running in the PI's group, but the system does not include any analytics. The HDS project, however, requires at least basic spectroscopic sample characterization, i.e., we could not really utilize the 2nd UHV system for this purpose so far. Thanks to supplemental funding of the prior grant, we installed a 2nd-hand AES/XPS system utilizing a CMA (cylindrical mirror analyzer) in the scattering chamber of the molecular beam system (see Fig. 4). The system is operational (see Fig. 5A/B). This allowed us to move the retarding field Auger system originally mounted on the beam scattering apparatus to the kinetics vacuum chamber. Thus, thanks to the supplemental funding, we have now two fully operational vacuum systems equipped with at least basic analytics. However, we were able to upgrade the system only after the supplemental funding came in (late in 2009).

In addition, the PI's group was engaged in setting up a time of flight system (Fig. 6) and an atmospheric flux reactor (Fig. 7). Both systems are operational. Furthermore, the molecular beam nozzle system has been upgraded, allowing it to reach greater nozzle/gas temperatures and impact energies. A gas mixing manifold to generate seeded beams more conveniently is also operational. These system upgrades resulted in a loss of measuring time but served to prepare for future projects. XPS, TOF, and the GC-based powder mini-reactor are essential components of the renewal grant.

When the acceptance notification for this grant arrived by e-mail in the PI's office, we were in the very final stages of a kinetics project on carbon nanotubes (CNTs). We took the opportunity to acknowledge this DoE grant in three publications concerning gas-surface interactions with CNTs.[8-10] Later, a review and invited conference paper were also related to the CNT work.[11, 12] However, the PI's group is not working on CNTs anymore.
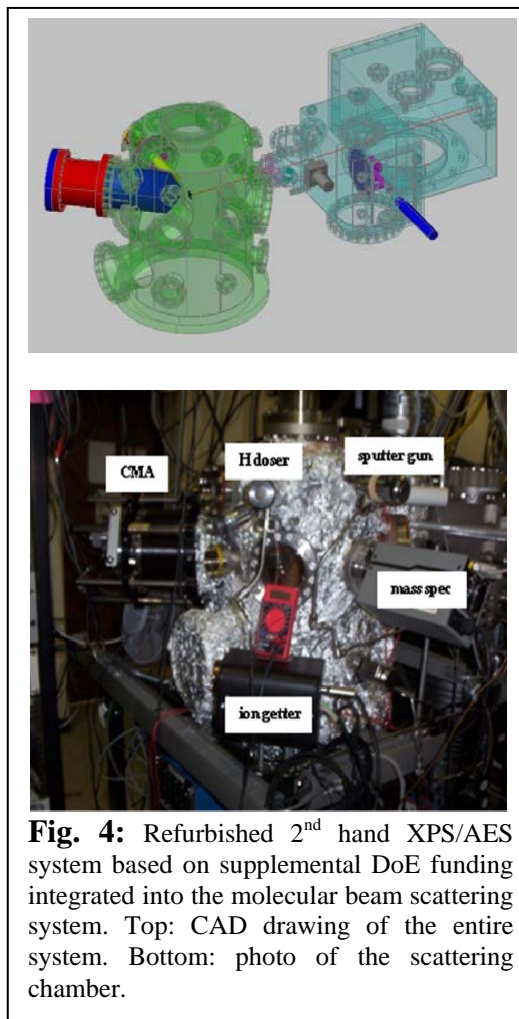

Fig. 4: Refurbished 2nd hand XPS/AES system based on supplemental DoE funding integrated into the molecular beam scattering system. Top: CAD drawing of the entire system. Bottom: photo of the scattering chamber.

6. Publications acknowledging the prior projects

Characterization of fundamental catalytic properties of MoS$_2$/WS$_2$ nanotubes and nanoclusters for desulfurization catalysis – a surface chemistry study

Additional PIs: none
Postdocs: Evgueni Kadossov (up to Dec. 2010), Junjun Shan (since Jan 2011)
Students: Mallikharjuna Komarneni (current), J. Goering (graduated)
Undergraduate students: Andrew Sand (chemistry, graduated in 2010 and joined the graduate school of the University of Chicago), Philip Nevin (biotechnology, 2009 summer exchange student from Sweden, joined the graduate school of Northeastern University in 2010), Razdan Mahalakshmi (biotechnology, joined grad. school in New York in 2009), John Justin (chemistry, 2009/10), Jordan Schmidt (physics, 2010)
Collaborators: M. Lu (Brookhaven National Laboratory – SEM sample characterization); B.W. Arey (Pacific Northwest National Laboratory – SEM sample characterization); R. Tenne, A. Zak, O. Eidelman (Weizmann Institute of Science, Israel – nanomaterials fabrication); L. Monica Veca (grad. student), Ya-Ping Sun (Clemson University)

Patent acknowledging DE-FG02-08ER15987 and NSF CAREER

P1) *METAL NANOPARTICLE DEPOSITED INORGANIC NANOSTRUCTURE HYBRIDS, USES THEREOF AND PROCESSES FOR THEIR PREPARATION,*
US Patent application #61/619,080, submitted,
by R. Tenne, Y. Tsverin, U. Burghaus, Mallikharjuna Rao Komarneni

Publications (2009-2011) acknowledging DE-FG02-08ER15987

1) *Adsorption of thiophene on inorganic MoS$_2$ fullerene-like nanoparticles*, **Catalysis Letters** <u>129</u> (2009) 66-70, by M. Komarneni, A. Sand, U. Burghaus

2) *Adsorption and reaction kinetics of small organic molecules on WS$_2$ nanotubes: an ultra-high vacuum study*, **Chemical Physics Letters** <u>479</u> (2009) 109-112, by M. Komarneni, A. Sand, P. Nevin, A. Zak, U. Burghaus

3) *Adsorption of thiophene on silica supported Mo clusters,* **Surface Science** <u>604</u> (2010) 1221-1229 by M. Komarneni, E. Kadossov, J. Justin, M. Ming, U. Burghaus

4) *Bond activation in thiophene and catalyst poisoning – nanosize Mo clusters supported on silica for desulfurization catalysis*, **Am. Chem. Soc., Div. Fuel Chem. <u>55</u> (2010) 594**, by E. Kadossov, M. Komarneni, J. Justin, U. Burghaus

5) *Reactive and non-reactive interactions of thiophene with WS$_2$ fullerene-like nanoparticles: an ultra-high vacuum surface science study*, **Catalysis Letters** <u>125</u> (2008) 236–242, by J. Goering, U. Burghaus, B.W. Arey, O. Eidelman, A. Zak, R. Tenne

6) *Multi-site kinetic Monte Carlo simulations of thermal desorption spectroscopy data*, **Surface Science** <u>603</u> (2009) 2494-2501, by E. Kadossov and U. Burghaus

7) *Short review: Surface science perspective of carbon dioxide chemistry - adsorption kinetics and dynamics of CO_2 on selected model surfaces,* **Catalysis Today** <u>148</u> (2009) 212-220, by U. Burghaus (invited and peer-reviewed)

8) *Adsorption kinetics of small organic molecules on thick and thinner layers of carbon nanotubes,* **Chemical Physics Letters** <u>470</u> (2009) 300-303, by M. Komarneni, A. Sand, M. Lu, U. Burghaus

9) *Possible effect of carbon nanotube diameter on gas-surface interactions – the case of benzene, water, and n-pentane adsorption on SWCNTs at ultra-high vacuum conditions,* **Chemical Physics Letters** <u>476</u> (2009) 227-231, by M Komarneni, A. Sand, J. Goering, U. Burghaus, M. Lu, L. Monica Veca, Ya-Ping Sun

10) *Adsorption kinetics of methanol on carbon nanotubes revisited – solvent effects and pitfalls in ultra-high vacuum surface science experiments,* **Chemical Physics Letters** <u>473</u> (2009) 131-134, by J. Goering, M. Komarneni, A. Sand, U. Burghaus

11) *Gas-carbon nanotubes interactions: a review of ultra-high vacuum surface science studies on CNTs,* **book chapter**, chapter 1 (pages 1- 56) in: Carbon Nanotubes: New Research, Avery P. Ottenhouse (Ed.), Nova Science, Inc. (NY), 2009, ISBN 978-1-60692-236-1, by U. Burghaus

12) *Effect of carbon nanotubes crystal structure on adsorption kinetics of small molecules – an experimental study utilizing ultra-high vacuum thermal analysis techniques*, conference proceedings (9 pages), invited (40 min) talk at the 38th NATAS conference, North American Thermal Analysis Society, Philadelphia, 2010, by Uwe Burghaus is additionally printed by Elsevier in **Journal of Thermal Analysis** <u>106</u> (2011) 123-128

13) *Nanotechnology for Sustainable Energy and Fuels*, conference report about this session of the ACS meeting in Boston, 2010, published as a Focus article in ACS Nano, invited (and edited), **ACS Nano <u>4</u> (2010) 5517-5526,** by Chang-jun Liu, Uwe Burghaus, Flemming Besenbacher, and Zhong Lin Wang

14) *Short review: site-specific surface chemistry on nanotubes,* **Israel Journal of Chemistry**, **<u>50</u> (2010) 449–452**, by U. Burghaus, A. Zak, and R. Rosentsveig (invited and peer-reviewed)

15) *New and future developments in catalysis: activation of carbon dioxide*, S.L. Suib (Editor), A. Koch (Senior Editorial Project Manager at **Elsevier**), **book chapter**, *Surface Science Studies of Carbon Dioxide Chemistry,* by U. Burghaus, submission deadline Dec. 2011

Additional publications (2009-2011) acknowledging supplemental equipment funding DE-FG02-08ER15987 (project co-funded by NSF CAREER)

16) *Adsorption dynamics of CO on copper and gold clusters supported on silica – how special is nanogold?,* **Chem. Phys. Lett.,** <u>517</u> (2011) 59-61, by J. Shan, M. Komarneni, and U. Burghaus

17) *Adsorption dynamics of CO on silica supported CuOx clusters – utilizing electron beam lithography to study methanol synthesis model systems,* **Journal of Physical Chemistry C,** <u>116</u> (2012) 5792–5801 by M. Komarneni, J. Shan, A. Chakradhar, E. Kadossov, S. Cabrini, U. Burghaus

Additional publications (2009-2011) acknowledging supplemental equipment funding DE-FG02-08ER15987 (project co-funded by DoE EPSCoR)

18) *Adsorption and dissociation kinetics of alkanes on CaO(100),* **Surface Science** <u>605</u> (2011) 1534-1540, by A.Chakradhar, Y. Liu, J. Schmidt, E. Kadossov, and U. Burghaus

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5. J. Goering, U. Burghaus, B.W. Arey, O. Eidelman, A. Zak ,R. Tenne, Catal. Lett. 125 (2008) 236-242
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9. M. Komarneni, A. Sand, J. Goering, U. Burghaus, M. Lu, M. Veca ,Y.-P. Sun, Chem. Phys. Lett. 476 (2009) 227-231
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11. U. Burghaus, (2009) Gas-carbon nanotubes interactions: a review of ultra-high vacuum surface science studies on CNTs, in Carbon nanotubes - Research Trends, Nova Science (New York), ISBN 978-1-60692-236-1
12. U. Burghaus, (2010) conference proceedings, invited talk at the 38th NATAS conference, North American Thermal Analysis Society, Philadelphia
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15. **S.L. Suib(Ed.)**, Elsevier in preparation (2012) Chapter x, "Adsorption of CO2 on solid surfaces.", U. Burghaus
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