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1. Capturing CO₂ from ambient air using a polyethyleneimine–silica adsorbent in fluidized beds

6 September 2014

Wenbin Zhang | Hao Liu | Chengong Sun | Trevor C. Drage | Colin E. Snape

Carbon Capture and Storage (CCS) uses a combination of technologies to capture, transport and store carbon dioxide (CO₂) emissions from large point sources such as coal or natural gas-fired power plants...



2. Engineering molecular dynamics simulation in chemical engineering

6 January 2015

Ji Xu | Xiaoxia Li | Chaofeng Hou | Limin Wang | Guangzheng Zhou | Wei Ge | Jinghai Li

Chemical engineering systems usually involve multiple spatio-temporal scales, grouped into different levels, from the molecular scale of reactants to the industrial scale of reactors. Molecular dynamics...



3. Discrete particle simulation of particulate systems: A review of major applications and findings

1 December 2008

H.P. Zhu | Z.Y. Zhou | R.Y. Yang | A.B. Yu

Understanding and modelling the dynamic behaviour of particulate systems has been a major research focus worldwide for many years. Discrete particle simulation plays an important role in this area....



4. Detailed numerical simulations of catalytic fixed-bed reactors: Heterogeneous dry reforming of methane

27 January 2015

Gregor D. Wehinger | Thomas Eppinger | Matthias Kraume

Highly endothermic (or exothermic) heterogeneous catalytic reactions are performed commonly in fixed-bed reactors with small tube-to-particle-diameter ratios N both in industrial and lab-scale applications....



5. Micromixers—a review on passive and active mixing principles

April–May 2005

Volker Hessel | Holger Löwe | Friedhelm Schönfeld

A review on microstructured mixer devices and their mixing principles concerning miscible liquids (and gases) is given. This is supplemented by the description of typical mixing element designs, methods...



6. Prediction of the crystal structures of axitinib, a polymorphic pharmaceutical molecule

6 January 2015

Manolis Vasileiadis | Constantinos C. Pantelides | Claire S. Adjiman

Organic molecules can crystallize in multiple structures or polymorphs, yielding crystals with very different physical and mechanical properties. The prediction of the polymorphs that may appear in...



7. Modelling and optimisation of the one-pot, multi-enzymatic synthesis of chiral amino-alcohols based on microscale kinetic parameter determination

27 January 2015

L. Rios-Solis | P. Morris | C. Grant | A.O.O. Odeleye | H.C. Hailes | J.M. Ward | P.A. Dalby | F. Baganz | G.J. Lye

Advances in synthetic biology are facilitating the de novo design of complex, multi-step enzymatic conversions for industrial organic synthesis. This work describes the integration of multi-step enzymatic...



8. Recent advances on membranes and membrane reactors for hydrogen production

5 April 2013

Fausto Gallucci | Ekain Fernandez | Pablo Corengia | Martin van Sint Annaland

Membranes and membrane reactors for pure hydrogen production are widely investigated not only because of the important application areas of hydrogen, but especially because mechanically and chemically...



9. CFD–DEM simulation of biomass gasification with steam in a fluidized bed reactor

27 January 2015

Xiaoke Ku | Tian Li | Terese Løvås

A comprehensive CFD–DEM numerical model has been developed to simulate the biomass gasification process in a fluidized bed reactor. The methodology is based on an Eulerian–Lagrangian concept, which...



10. Nanoparticle synthesis in microreactors

1 April 2011

Chun-Xia Zhao | Lizhong He | Shi Zhang Qiao | Anton P.J. Middelberg

Nanoparticles have been a research focus for more than two decades. The advent of microfluidic technology provides alternative strategies for the synthesis of nanoparticles in reactors having a micrometer...



11. Multiscale molecular modeling can be an effective tool to aid the development of biomass conversion technology: A perspective

6 January 2015

Samir H. Mushrif | Vallabh Vasudevan | Chethana B. Krishnamurthy | Boddu Venkatesh

Lignocellulosic biomass is an alternate and renewable source of carbon. However, due to high oxygen content and diverse functionality, its conversion to fuels and chemicals is technologically challenging....



12. Discrete particle simulation of particulate systems: Theoretical developments

July 2007

H.P. Zhu | Z.Y. Zhou | R.Y. Yang | A.B. Yu

Particle science and technology is a rapidly developing interdisciplinary research area with its core being the understanding of the relationships between micro- and macroscopic properties of particulate/granular...



13. Adsorption of CH₄ and CH₄/CO₂ mixtures in carbon nanotubes and disordered carbons: A molecular simulation study

6 January 2015

Lang Liu | David Nicholson | Suresh K. Bhatia

We report a comparison of the adsorption of CH₄ and CO₂/CH₄ mixtures of different composition in three different types of nanoporous carbons including carbon nanotubes, and activated carbon fibre (ACF-15)...



14. Scalability of mass transfer in liquid–liquid flow

6 September 2014

A. Woitalka | S. Kuhn | K.F. Jensen

We address liquid–liquid mass transfer between immiscible liquids using the system 1-butanol and water, with succinic acid as the mass transfer component. Using this system we evaluate the influence...



15. Cellulose dissolution and regeneration in ionic liquids: A computational perspective

6 January 2015

Krishna M. Gupta | Jianwen Jiang

To meet the increasing global energy demand and reduce the dependency on traditional fossil fuels, renewable biomass particularly cellulose has attracted considerable interest. Prior to processing and...



16. Production of recombinant proteins by high cell density culture of *Escherichia coli*

February 2006

Jong Hyun Choi | Ki Chang Keum | Sang Yup Lee

Escherichia coli has been the most widely used host for the production of recombinant proteins because it is the best characterized system in every aspect. Furthermore, the high cell density culture...



17. Insight into the nucleation of urea crystals from the melt

6 January 2015

Federico Giberti | Matteo Salvalaglio | Marco Mazzotti | Michele Parrinello

Obtaining molecular-level information regarding nucleation is an essential step towards a thorough comprehension of crystallization processes. In this work we investigate the nucleation of urea at the...



18. MOF-74 building unit has a direct impact on toxic gas adsorption

15 January 2011

T. Grant Glover | Gregory W. Peterson | Bryan J. Schindler | David Britt | Omar Yaghi

Metal organic framework (MOF-74) analogs have been synthesized using cobalt, magnesium, nickel, and zinc metal centers. The capability of these materials to remove ammonia, cyanogen chloride, and sulfur...



19. Enhancement effect of lithium-doping functionalization on methanol adsorption in copper-based metal-organic framework

17 February 2015

Ying Wu | Defei Liu | Huiyong Chen | Yu Qian | Hongxia Xi | Qibin Xia

Grand canonical Monte Carlo (GCMC) simulations combined with density functional theory (DFT) calculations were performed to evaluate the functionality effect of Li-doping on methanol adsorption over...



20. Modelling reactive distillation

November 2000

R. Taylor | R. Krishna

The design and operation issues for reactive distillation systems are considerably more complex than those involved for either conventional reactors or conventional distillation columns. The introduction...



21. Microfluidics for medical diagnostics and biosensors

1 April 2011

Catherine Rivet | Hyewon Lee | Alison Hirsch | Sharon Hamilton | Hang Lu

This article reviews the recent development in microfluidics for medical diagnostics and integrations with biosensors. Diagnostic and sensing applications have been the focus of much of the development...



22. Perspectives on molecular simulation of clathrate hydrates: Progress, prospects and challenges

6 January 2015

Niall J. English | J.M.D. MacElroy

In this review, the intriguing properties of clathrate hydrates shall be discussed, as well as their environmental impact and prospects for energy exploitation in industry. In particular, the anomalous...



23. Base promoted hydrogenolysis of lignin model compounds and organosolv lignin over metal catalysts in water

17 February 2015

Hannelore Konnerth | Jiaguang Zhang | Ding Ma | Martin H.G. Precht | Ning Yan

Herein we present a systematic investigation on the promotional effect of base in metal catalysed hydrogenolysis of lignin model compounds and organosolv lignin. The research started with the evaluation...



[24. Assembly engineering: Materials design for the 21st century \(2013 P.V. Danckwerts lecture\)](#)

6 January 2015
Sharon C. Glotzer

We introduce the emerging discipline of Assembly Engineering and its role in the design and synthesis of new materials for next generation applications. We especially highlight the role of computer...



[25. High-fidelity simulation of the 3-D full-loop gas–solid flow characteristics in the circulating fluidized bed](#)

17 February 2015
Kun Luo | Fan Wu | Shiliang Yang | Mingming Fang | Jianren Fan

The full-loop gas–solid motions in a three-dimensional circulating fluidized bed are numerically modeled using the computational fluid dynamics combined with the discrete element method. The time-averaged...

