Topical Sessions

1 MODELING IN MATERIAL SCIENCE

Monday, 21.06.2010, Room 115

Time	ID	MODELING IN MATERIAL SCIENCE I *Chair: E. Kaxiras, EPFL*
13:30	101	**Au(111) vicinals reconstruction pattern and steps as nanostructure template: an atomistic insight** *Roberto Gaspari, Carlo Antonio Pignedoli, Daniele Passerone, Roman Fasel, EMPA, Überlandstrasse 129, 8600 Dübendorf* Using classical and ab initio simulations, we study the interplay between Au(111) surface reconstruction and the presence of steps on a vicinal face. The experimentally observed patterns are reproduced and explained, and a complete description of the structure of this vicinal is given, paving the way to the production of accurate templates for molecular self-assembled nanostructuring.
13:45	102	**Chemical reactivity on surfaces** *Stephan Blankenburg [1], Eva Rauls [2], Wolf Gero Schmidt [2]* *[1] EMPA, Überlandstraße 129, 8600 Dübendorf* *[2] Universität Paderborn, Pohlweg 55, DE-33100 Paderborn* Supramolecular architectures created by self-organization of organic molecules adsorbed on metal surfaces are a field of intense research [1]. Especially peptide bonding is a promising mechanism for controlled structure design. We have studied the formation of covalently bonded networks formed by 4,4'-diamino-p-terphenyl (DATP) and 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) on Au(111) [2] and by 1,3,8,10-tetraazaperopyrene (TAPP) on Cu(111) [3] by means of density functional theory. The surface has been found to significantly modify the thermodynamics and reaction barriers of both covalent syntheses. While the formation of the surface-supported polymerization of DATP and PTCDA can be traced to dispersion interactions and molecular strain [4], the coupling of TAPP is mainly driven by a transition state determined by a covalent bond to the substrate. Here, mobile adatoms play an important role [5]. [1] J. A. A. W. Elemans, S. Lei and S. DeFeyter, Angew. Chem. Int. Ed. 48, 7298 (2009). [2] M. Treier, N. V. Richardson and R. Fasel, J. Am. Chem. Soc. 130, 14054 (2008). [3] M. Matena, T. Riehm, M Stöhr, T. A. Jung and L. H. Gade, Angew. Chem. 120, 2448 (2008). [4] E. Rauls, S. Blankenburg and W. G. Schmidt, PRB B 81,125401 (2010). [5] S. Blankenburg, E. Rauls and W. G. Schmidt, PRL, submitted (2010).

14:00	103	**Bottom-up modeling of the elastic properties of organosilicate glasses and their relation to composition and network defects**

Jan M. Knaup [1], Efthimios Kaxiras [1], Li Han [2], Joost J. Vlassak [2]
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Organosilicate glasses (OSG) are used as low-k inter metal dielectrics for advanced integrated circuits. In this application, the material must fulfill two conflicting requirements, on the one hand it has to have a low density to reduce the dielectric constant, on the other hand it has to be mechanically stable enough to withstand the thermally induced stress arising during subsequent steps of integrated circuit manufacture. Recent experimental advances in improving the mechanical and electrical properties of these materials have, however, not yet been systematically studied theoretically on an ab initio level. In this work, we employ the very efficient density-functional based tight-binding (DFTB) method to achieve an accurate description of OSG of different compositions with perfect and defective network coordination. Our results show, that a transition between different mechanisms of elastic deformation between silica glass and silicon hydrocarbide leads to different behaviors of the density, stuffness and sensitivity to network defects depending on the hydrocarbon content.

14:15	104	**All-atom molecular dynamics simulations of amorphous, crosslinked PDMS**

Philip T. Shemella [1], Teodoro Laino [1], Alessandro Curioni [1], Oliver Fritz [2]
[1] IBM Research – Rüschlikon
[2] ABB Research - Dättwil

The structure, dynamics, and self-diffusion properties of amorphous, binary mixture of large poly(dimethylsiloxane) (PDMS) and small poly(hydromethylsiloxane) (PHMS) are characterized with atomic-level molecular dynamics simulations. Molar masses and mixing properties are comparable and relavant to commerical products, and simulations require massively parallel molecular dynamics simulations. The system consists of 100 vinyl-terminated PDMS molecules (~72,500 g/mol) and 200 crosslinker PHMS molecules (~1960 g/mol), for a total of more than 1 million atoms. Molecular diffusion is studied as a function of temperature, electric field, and end-crosslinking density. Simulation results provide an atomic-level description for molecular motion and an understanding of the local structure that contributes to molecular self-diffusion.

14:30	105	**Convergent Space Sampling by Deduction and Induction from Material Sciences to Bio-Structural Chemistry**

Christian Lehmann, EPFL-LTP-IMX-STI, CH-1015 Lausanne

The presence of a solid phase irregularity termed "screw dislocation" proved not only the clue to an ingenious theory of F. C. Frank to explain the observed high growth rates of crystals, but also led J. D. Watson and F. C. Crick to postulate the most influential paradigm of structural molecular biology: helical arrangement principles in TMV virus assembly and in DNA, more than half a century ago. The controlled nucleation of 'cosy corners' to initiate a first helical turn has by now been achieved for peptide α-helices, but also for left- and right-handed chiro-sensitive synthetic nucleic acids and a number of further molecular biological targets, making

		essential use of a suitable force field (MAB) and a program suite (MOLOC) developed in the context of pharmaceutical chemistry. A conformational space sampling algorithm proves not only useful for the optimization of inhibitor-receptor recognition, but also to determine the preferred binding sites and conformations of organic molecules on defined mineral surfaces. Helical polymers derived from extended pyrromethenes ("porphohelicenes") and nucleic acids with strongly dipolar chromophores offer themselves as potentially conducting polymers, their systematic exploitation however remains in the blueprint.

14:45	106	**Large scale computer simulations of strain distribution and electron effective masses in silicon <100> nanowires**

Christian Tuma, Alessandro Curioni
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A new multiscale method is proposed to analyze the internal redistribution of tensile strain applied to silicon <100> nanowires and its effect on electron effective masses m^*. Non-periodic, realistic models of unprecedented size containing up to 2.2×10^7 atoms ($652 \times 26 \times 26$ nm^3) allow the identification of non-uniform redistribution patterns specific to the constraints applied to impose external strain. Depending on how the external strain is imposed, silicon nanowires can show m^* behavior similar to strained bulk silicon, or, as a function of nanowire size, can display intrinsic strain large enough that external strain hardly reduces m^* further. For nanowire cross section sizes smaller than 8×8 nm^2 quantum confinement leads to an increase in m^* which cannot be compensated for by tensile strain [1].

[1] C. Tuma, A. Curioni, Appl. Phys. Lett. (2010) accepted for publication

15:00	123	**Optical response of gold and its alloys studied with DFT and beyond-DFT methods** *(changed from poster to talk)*

Deniz Keçik [1], Helena Van Swygenhoven [1], Efthimios Kaxiras [2]
[1] Materials Science and Simulation, NUM/ASQ, PSI, 5232 Villigen PSI
[2] EPFL-STI-IMX-LMMM, MXC 337, Station 12, 1015 Lausanne

Density functional theory (DFT) is a powerful technique to calculate the bandstructure and dielectric function of metals and alloys. In this study the optical reflectivities of gold-based alloys via DFT and some beyond-DFT methods are calculated. One can obtain information about the crucial optical excitations (specifically the nature of interband transitions) and absorption edges (thus the major change in reflectivities) from bandstructures and dielectric functions of the considered systems. We used the ab initio package VASP for standard LDA/GGA calculations on pure Au, Ag, Cu and Al metals as well as some randomly configured (Au-Ag and Au-Al) and ordered intermetallic alloys (Au(Al,In,Ga)$_2$). The ultimate goal of the study is to investigate if there is a reasonable trend in the optical absorption edges as a function of impurity additions and if the calculations can be used to predict color trends.

The results of fully relativistic GGA calculations show that qualitatively there is a quite good agreement in the reflectivity spectra of pure and impurity-added systems between our results and some experimental reference data. However, quantitatively the rapid drop in reflectivity below a particular wavelength for pure metals differs from experiments by up to 100-200 nm. For the intermetallics AuAl$_2$ and AuGa$_2$, the central dip in reflectivity agrees qualitatively well with some experiments. Although standard DFT preserves its role as a guide for understanding the mechanisms in optical response of our metallic systems, we cannot disregard its shortcomings such as inaccuracies in band energy differences, being a ground state theory. There

red		are several cures suggested to this problem, one of them being the inclusion of a small fraction of the non-local exchange in the Hamiltonian (hybrid functionals). We intend to present here also the results of hybrid functional calculations, on a comparative basis with the outcome of standard DFT simulations.
15:15		*Discussion, first chance to look at posters and make contacts*
15:30		***Coffee Break***
		MODELING IN MATERIAL SCIENCE II *Chair: H. Van Swygenhoven-Moens, PSI,* *A. Curioni, IBM Rüschlikon*
16:00	111	**Iron EAM potential and magnetism: results of an extensive fitting attempt.** *Samuele Chiesa [1], Peter Derlet [1], Mark Gilbert [2], Sergei Dudarev [3], Helena Van Swygenhoven [1]* *[1] Paul Scherrer Institute, 5232 Villigen PSI* *[2] University of Oxford, OxfordMaterials, Oxford OX1 2JD, UK* *[3] Culham Centre for Fusion Energy, Abingdon, Oxfordshire OX14 3DB, UK* The Dudarev-Derlet potential is a way to incorporate zero temperature magnetism in a second moment EAM formalism. We report on an extensive effort to fit spin-polarized DFT predictions of pure iron to this magnetic potential formalism. A comparison with recent semi-empirical potentials for bcc iron shows that the main (and common) fitting difficulties concern the zero temperature fcc phase and the screw dislocation migration mechanism. For instance the energy difference between the non-magnetic and ferromangetic fcc phase is strongly overestimated, but how this relates to the description of the thermally activated bcc-fcc phase transition cannot be easily answered. The screw migration mechanism is still an open question and will be discussed within the framework of the string-potential formalism for the core structure of a screw dislocation.
16:15	113	**Modelling Fe-Cr alloys by first-principle calculations and EXAFS measurements** *Anne-Christine Uldry, Camelia Borca, Andi Idhil, Maximo Victoria, Wolfgang Hoffelner, Maria Samaras, Paul Scherrer Institut, 5232 Villigen PSI* The modelling of Fe-Cr alloy has been the object of intense activities in recent years in view of the possible use of these compounds as structural materials for the next generation of nuclear reactors. The basis of multiscale approaches to material modelling are usually Density Functional Theory (DFT) calculations, which allow the determination of the basic interactions in the material from first principles. It is therefore crucial that direct validations of the model at this level of modelling are performed. Synchrotron X-ray experiments offer a means to compare measured quantities with calculated ones. The Extended X-ray Absorption Fine Structure (EXAFS) technique in particular is extremely sensitive to the structural environment in the first shells of a give atomic species. Fitting the EXAFS results can therefore be used as a method to discriminate between different models and atomic arrangements. A series of supercell DFT calculations for the pure Fe-Cr alloy in the concentrations 6.3, 9.3, 12.5 and 16 at% Cr have been performed by varying the respective configurations of Fe and Cr for each given concentration and using the total energy as selecting criterion. EXAFS measurements on model Fe-Cr alloys with up to 16% Cr content were taken at the microXas beamline of the PSI Swiss Light Source. We

		will show that the combination of DFT modelling and EXAFS measurements is a powerful tool to investigate the cross-over from a tendency to short-range order to a tendency to cluster exhibited by the Fe-Cr alloy around the 10-12 at% Cr concentration.
16:30	**114**	**Embrittlement of Ni** *Georg Schusteritsch [1,2], Efthimios Kaxiras [1]* *[1] Laboratory for Multiscale Modeling of Materials, EPFL* *[2] School of Engineering and Applied Sciences, Harvard University, Cambride MA, USA* The embrittlement of Ni due to the presence of S impurities is studied using first principles density-functional-theory calculations, which are treated in the context of Rice's theory based on generalized-stacking-fault energetics and the unstable stacking energy criterion. Our density-functional-theory calculations are used to determine the ductility parameter $D = \gamma_s / \gamma_{us}$. This ratio of the surface energy γ_s to the unstable stacking energy γ_{us} enables us to study the effect of embrittlement for both bulk Ni with substitutional S impurities and for a $\Sigma5(012)$ grain boundary (GB) with interstitial S impurities. We are able to show that the inclusion of S impurities increases the value of the ductility parameter D by 41% in bulk Ni. In contrast, the ductility parameter D is reduced by 85% for the GB. These results strongly suggest that such embrittlement of Ni is related to the effect of the S impurities on grain boundaries.
16:45	**115**	**Modeling recovery and creep by discrete dislocation dynamics** *Péter Dusán Ispánovity [1], István Groma [2], Maria Samaras [1], Wolfgang Hoffelner [1]* *[1] Paul Scherrer Institut, 5232 Villigen PSI* *[2] Eötvös University Budapest, Pázmány Péter sétány 1/a., HU-1117 Budapest* The formation and evolution of the subgrain (or cell) structure that develops at high temperatures in crystalline materials has been subject of increasing interest. Beside its effect on mechanical properties, it also plays an important role in, e.g., nucleation of recrystallization. Since subgrain boundaries consist of individual dislocations, we propose to study the microstructure evolution by 2D discrete dislocation dynamics simulations. We show that in the case of recovery (zero external stress), the model is able to reproduce several experimentally observed features of subgrain coarsening, such as abnormal growth, power-law kinetics and the temperature dependence of the power-law growth exponent. When a small external stress is applied (creep), the system reaches a steady-state, which is characterized by constant strain rate and a microstructure in dynamic equilibrium (with constant subgrain size). The strain rate follows a Norton-type law. This is also in agreement with the experimental findings.
17:00	**116**	**Multi-scale modeling of radiation induced defect structure evolution using stochastic differential equations** *Peter Derlet, Cond. Matter Theory Group, Paul Scherrer Institut, 5232 Villigen PSI* *Sergei Dudarev, Theory and Modelling Department, Culham Centre for Fusion Energy, Abingdon, Oxfordshire OX14 3DB, UK, United Kingdom* Materials under extreme irradiation conditions form complex and evolving dislocation and defect microstructure that can significantly affect the mechanical response of a material. Damage created by either neutron or ion irradiation create vacancy and interstitial based defects that are highly mobile, and strongly interacting with each

other and the surrounding existing dislocation network. On the one hand, in the far-field limit, the interaction is elastic and therefore amenable to linear (anisotropic or isotropic) elasticity. On the other hand in the near field limit, corresponding to an atomic scale, understanding is necessary to properly model their interaction, as well as their mobility and any possible reaction process. Such an environment is therefore a multi-scale phenomenon and careful consideration must be given to develop the optimal modeling strategy. In the present contribution, the use of stochastic many-body differential equations is considered as an alternative to traditional atomistic molecular dynamics methods and the more mesoscopic methods based on the kinetic Monte Carlo method that are currently used to model such microstructural evolution. The main objective of the work is the development of a fast algorithm for predicting the mechanical response of a material resulting from microstructural evolution driven by interacting radiation defects formed in a material under fission and fusion operating conditions in the next generation commercial and experimental reactors.

17:15	**117**	**Modeling of the rheological behaviour of an Al-Cu alloy during solidification using a discrete/finite element procedure**

M. Sistaninia [1], A. B. Phillion [1,2], J.-M. Drezet [1], M. Rappaz [1]
[1] Computational Materials Laboratory, EPFL
[2] School of Engineering, University of British Columbia Okanagan, Kelowna, Canada

The rheological behaviour of an Al- 2wt%Cu alloy at a given solid fraction is modelled using a combined Finite Element / Discrete Element procedure. A 3D solidification model is used for generating the geometry of the semi-solid microstructure. The solidification model is based on a Voronoi tessellation of randomly distributed nucleation centres and a solute diffusion model for each element of this tessellation. The solid grains are modelled using Norton-Hoff viscoplastic constitutive law. The connectivity between grains prior to coalescence is modelled using connector elements, each consisting of one spring and one damper acting in parallel to approximate the intergranular liquid phase. The model predictions are validated against experimental data from the literature. The results show that a combined FE / DEM simulation is a good tool for modeling the rheological behaviour of semi-solid alloy for solid fractions higher than 0.90, with account of the localisation of strains and stresses.

17:30	**118**	**Laue diffraction spots obtained from 3D dislocation dynamic simulations**

Jorge Martinez Garcia [1], Helena Van Swygenhoven-Moens [1], Jochen Senger [2], Daniel Weygand [2]
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White beam Laue diffraction is nowadays a well-established technique for studying the microstructure of materials. Valuable information on the dislocation distributions appearing in the sample during plastic deformation, for instance, can be directly inferred from the shape and position of the diffraction spots. So far the experimentally observed features of the spots (i.e. streaking and splitting) has been explained on the basis of simple dislocations models, assuming random distributions of straight-line dislocations. In the present work, we attempt instead to describe the main features of Laue diffraction spots calculated from dislocation arrangements generated by 3D dislocation dynamics simulations as well as to discuss the main potentiality of this new computational approach.

17:45	119	**Multiphase-field simulation of micropores constrained by a solid network: The pinching effect**

H. Meidani, A. Jacot, M. Rappaz
Computational Materials Laboratory, EPFL, Station 12, 1015 Lausanne

Microporosity is one of the major defects encountered in solidification processes. It considerably deteriorates the mechanical properties of cast parts, in particular fatigue life. The pore morphology, namely the curvature distribution, can substantially influence the gas pressure inside the pore and therefore the pore size. In recent X-ray tomography observations, mean curvatures larger than 0.2 μm^{-1} were observed, which corresponds to a Laplace–Young overpressure of more than 400 kPa.

The novelty of the current study is the application of a multiphase-field modeling approach, which allows for direct description of the morphology of a pore in contact with solid and liquid phases. The method accounts for the pressure difference between the liquid and gas phases, as well as diffusion of dissolved gases in the liquid. The model incorporates the perfect gas and Sievert's laws to describe the concentration and partitioning of the dissolved gas at the pore/liquid interface. The model was used to study the pinching effect, i.e. the geometrical constraint of the dendritic solid network on the pore morphology. The results were compared with models available in the literature. It is shown that a direct description of the pores can provide new insights into the pinching effect and the morphology of the micropores, by the fact that it allows for the incorporation of additional physics such as unequal interfacial energies.

18:00		*END*
18:30		*Postersession, Apéro, Barbecue*

ID	MODELING IN MATERIAL SCIENCE POSTER
121	**Applications of graphene-based nano-structures produced by bottom-up technologies**

Stephan Blankenburg, Daniele Passerone, EMPA, Überlandstraße 129, CH-8600 Dübendorf

The fabrication of membranes with a high selectivity on the nanometer scale is an emerging field of research. We investigate the possibility to use bottom-up approaches to construct a filter with porous graphene using first principle calculations. Here, the porous network is produced by the self-assembling of hexaiodo-substituted macrocycle cyclohexa-m-phenylene (CHP). The resulting porous network exhibits an extremely high selectivity up to 10^{23} (10^{10}) for H_2 (O_2) compared to other atmospheric molecules like O_2, N_2, CO, CO_2 and NH_3. Therefore, the results show that the presented membrane is superior to traditional filters using polymers or silica and could have a high potential for further technological applications like gas sensors or fuel cells.

122	**Experimental analysis and computational modeling of temperature dependent cyclic plastic hardening and strain controlled ratcheting**

Koenraad Janssens
Paul Scherrer Institute, Laboratory for Nuclear Materials, OVGA / 6, CH-5232 Villigen PSI

Cyclic temperature shock induced low cycle fatigue can play a role in the safety of the primary cooling system of nuclear reactor power plants. As the yield stress varies with temperature, a thermal shock leads to a sudden local change in the mechanical properties, which may

induce unrealistic strain localization and local ratcheting in an elasto-plastic finite element model. We present an experimental analysis of the temperature dependent cyclic hardening of AISI 316L stainless steel, and report on the influence of ratcheting as observed in strain-controlled fatigue experiments. An evaluation of the performance of an implementation of the experimental data into a temperature-dependent, cyclic plastic hardening model is given in the context of a case study of notched ring specimens submitted to cyclic thermal shocks.

124	**Atomistic modeling of carboxylate adsorption onto different aluminiumoxide and hydroxide surfaces**

Christian Lehmann, Abhishek Tewari, Sandra Galmarini, Paul Bowen
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The characterization of crystal surfaces in alumina polymorphs and their interaction with carboxylates is important both in ceramic processing and surface functionalization for biomedical applications. We have undertaken a comparative study for a series of crystal surfaces using a molecular design software (MOLOC) and ionic crystal energy minimization (METADISE). MOLOC is a molecular modeling suite based on the MAB force field as developed for use in bio-structural and pharmaceutical chemistry. In the present study, lowest energy manifolds for carboxylates (neutral and ionic form) were generated on different crystallographic faces: α-Al_2O_3, (001), (012); Boehmite (010) and Gibbsite, Bayerite and Nordstrandite (001) interstitial surfaces. Adsorption energies of the lowest energy positions were then estimated. The results show characteristic relative binding energies, for the different surfaces, which can be mainly attributed to their hydrogen bond strength and a weak dispersive interaction term. This simple systematic surface sampling method holds significant promise for design strategies for the functionalization and self-assembly of nanoparticles in numerous contexts.

125	**Dislocation loops in nanocrystalline metals**

Mario Augusto Velasco Sanchez, Christian Brandl, Helena Van Swygenhoven-Moens
Materials Science and Simulation, Paul Scherrer Institut, 5232 Villigen PSI

In a nanocrystalline grain boundary (GB) network dislocations usually nucleate at ledge structures in the GB and propagate throughout the grain, depositing dislocation line sections at the GBs. Recent simulations of nc-Al deforming at a constant strain rate have shown that the propagation of dislocations along GBs can be a rather complex process involving multiple cross-slip events to avoid depositing edge dislocation segments into locally compressive regions of the GB. Thus via cross-slip the dislocation is able to propagate along more favourable regions such as triple lines under tension.
Here we use the atomistic simulation methodology published in [MSMSE 17(2009)055008] to implement well-defined dislocation loops in a grain having well defined misorientations with its nanocrystalline environment. This allows to study the reaction of GBs when bombarded with several dislocations and this as function of their tilts and twist component.

112	**He atoms in BCC iron studied with molecular dynamics** *(changed from talk to poster)* *Ning Gao, Jiachao Chen, Max Victoria, Helena Van Swygenhoven* *Paul Scherrer Institute, 5232 Villigen PSI* Helium atoms can precipitate leading to swelling, often causing embrittlement. Predicting materials behaviour requires the understanding the interactions of helium with different defects, such as vacancies. The clustering of He in a Fe lattice and the nucleation of a He bubble have been studied with molecular dynamics simulations (MD). The binding energies are in good agreement with ab initio results, showing after 4~6 He atoms are inserted interstitially, the first interstitial being kicked out. After insertion of 16 He atoms, a <110> dumbbell of Fe is formed binding with He-V cluster. The He-V clusters can form regular lattice configurations depending on the number of He atoms: first a dumbbell He cluster is formed, growing to a tetrahedral structure and finally to structures close to fcc lattice. The stress around He-V cluster can be up to 9 GPa, which is lower than the empirical predication of 0.2μ.
126	**Adsorption, diffusion and coupling of phenyl groups on Cu(111):** **DFT calculations** *Manh-Thuong Nguyen, Daniele Passerone, EMPA, Überlandstrasse 129, 8600 Dübendorf* The overall coupling process of phenyl radicals – the important intermediates in the prototypal Ullmann reaction – on Cu(111) is addressed using density functional theory. It is found that a single phenyl group covalently binds to the substrate with the ring plane tilted 36° with respect to the surface. The phenyl group is very mobile on Cu(111), characterized by a very lower diffusion energy barrier of 0.09 eV. A total energy analysis shows that on the surface two phenyl groups attract each other. The coupling between the two reactants happens after they simultaneously bind to the same surface atom, the energy barrier is found to be 0.38 eV. All computational results are in good agreement with experimental data.
127	**First-principles study of copper-phthalocyanine complexes on graphene** *Jun Ren, Sheng Meng, Efthimios Kaxiras* *Laboratory for Multiscale Modeling of Materials, Institute of Materials, EPFL* We have investigated the electronic interaction between copper hexadecafluorophthalocyanine ($F_{16}CuPc$) and epitaxial graphene, by using the firstprinciple calculations within the framework of density functional theory (DFT) as implemented in SIESTA code. The $F_{16}CuPc$ and graphene system is an important model system for future electronic and energy applications. We found that the molecules are physisorbed on graphene surface, lying flat and forming two well-ordered phases of incommensurate crystalline island. The ordering is dominated by moleculesurface and intermolecular van der Waals interactions, together with a small amount of charge transfer from the graphene to $F_{16}CuPc$ molecule. Consequently, the molecules are preferentially adsorbed on monolayer graphene when the monolayer and bilayer graphene coexist, due to the higher density of states at Fermi energy of the former. In addition, we identify a local characteristics of bilayer graphene layer at ~0.4 eV about the Dirac point, indicating that its electronic structure is modified upon molecular adsorption.