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How dense is the gas adsorbed in nanopores?

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Abstract

Unlike macroscopic objects, any system of nanometric size shows characteristics that strongly depend on its size and geometric form. It is mainly because the major part of atoms (or molecules) of nano-object is located at its surface, and their cohesive energy is smaller than for the atoms in the bulk. Here we show that when a fluid is confined in nano-volume, delimited by non-attractive pore walls, its density is heterogeneous, in particular close to the pore wall, and, on average, smaller than the density of bulk fluid. This effect progressively weakens when the pore size increases, and totally disappears for pores larger than 5 nm. The reported observation has non-trivial influence on evaluation of total and excess amount of fluid adsorbed in nanopores, as these quantities are traditionally calculated assuming the known – and homogeneous –density of the bulk fluid. Additionally, we propose a new method of the estimations of the accessible pore volume, based on the analysis of the density of confined fluid. The right estimation of both: pore volume and gas density is essential for quantitative interpretation of experimental adsorption isotherms: evaluation of pore size distribution and of the adsorbed amount. Although we analyze these problems taking an example of hydrogen at 77 K, our conclusions are general and apply to any fluid confined in nanopores.

Keywords: adsorption, Monte Carlo simulations, confined gas density, nanopores, hydrogen

1. Introduction

It is well know that the properties of nanoobjects differ from those of their macroscopic analogs. Any system of nanometric size shows characteristics which strongly depend on its size and geometric form. It is mainly because the major part of atoms (or molecules) of nano-volume are located at the object surface and their cohesive energy is smaller than for the atoms in the bulk. As a consequence, the properties of the nanoobjects are usually not homogeneous, and may vary with the distance from the object boundary.

It is also the case when fluids are adsorbed (or confined) in nanospaces. The attractive force field of the pore wall is a source of additional pressure that can attain the values as high as 1-10 GPa [1-2]. It induces the organization of confined fluid that is not observed in bulk systems at the same thermodynamic conditions [3-4].The influence of the wall progressively diminishes when the distance from the pore wall increases. In consequence the density of fluid inside a nanopores is heterogeneous.

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To the best of our knowledge, there are no detailed studies showing how the properties of fluids change when they are confined in nanospaces delimited by *non-attractive walls*. Only the density of the hard-sphere fluid against a hard wall was studied [5]. However, the analysis of fluid density variation under nano-scale confinement is missing. At the same time, the exact knowledge of the quantity of gas that can fill a given volume at the specific thermodynamic (p,T) conditions (N_{gas}) is essential when one has to convert the total amount (N_{tot}) of gas stored (adsorbed) in this volume into the excess amount (N_{exc}), or vice versa: $N_{exc} = N_{tot} - N_{gas}$. This conversion is always necessary when the experimental measurements of adsorption have to be model/interpret using computer simulations. In fact, from computer simulations the total amount of the gas adsorbed in a pore of a given size and shape is directly obtained, whereas in gravimetric experiment the excess amount is usually measured.

The exactness of the conversion relays on a correct evaluation of the quantity of gas that could occupy the same pore volume (N_{gas}). Therefore, the estimation of N_{gas} requires an exact knowledge of two parameters: (i) the volume of the pore accessible for adsorbate molecules (V_{access}), and (ii) the density of the gas at the given (p,T) conditions (ρ_{gas}). Both quantities are easy to define when the pores of the adsorbent are macroscopic. When the pore dimensions are of the order of few nanometers, the definitions of the volume of the nanopores accessible for adsorbate molecules (V_{access}) and the density of the gas that could be potentially confined (without being adsorbed) in such nanopores are not trivial.

The recent papers of D.D. Do et al. [6-7] have revisited the notion of volume accessible in nanopores and proposed a new definition based on the analysis of adsorbate-adsorbent interaction. In the present work we propose an alternative methodology, which is also a consequence of the balance between the adsorbate-adsorbent and adsorbate-adsorbate interactions. On the contrary, the question 'what is the density of a gas that could potentially be confined within a volume of nanometric size' has never got any attention. All experimental and theoretical studies assume that this density is homogeneous regardless the temperature and the size of confining reservoir, and equal to the density of bulk (3D) gas. We show in the present work that both assumption are not exact.

We limit our analysis here to a single case of hydrogen gas confined in non-adsorbing pores at 77K, but the conclusions have general character and apply to any fluid confined in nanopores. Two typical model pores geometries were investigated: infinite slit-shaped and cylindrical pores. We show that the distribution of hydrogen molecules confined by the non-adsorbing pore walls is not uniform, and that the average density of the confined gas is smaller than the density of macroscopic gas quantity at the same thermodynamic conditions. We focus our discussion on gas properties in micropores (of the width/radius smaller than 2 nm), but we show the results for the pore sizes up to 5 nm. For larger pores the influence of the heterogeneity of the gas distribution is negligible. The average density is dominated by the homogeneous contribution from bulk gas inside the pore.

2. Methods, and pore and interactions models

All calculations were performed using Monte Carlo method in grand canonical ensemble (GCMC). We have used our own code, extensively tested and validated in the past [8-11]. The simulations were carried out at constant temperature (T = 77 K), and hydrogen pressure (p) varying from 1 to 200 bar. The hydrogen pressures were converted into corresponding fugacities using van der Waals equation of state and NIST database [12]. At all (p,T) conditions studied in the present work the difference bettween fugacity and pressure of

hydrogen is small, but not negligeable (~10%). Therefore in GCMC simulations we have used the fugacity to calculate chemical potential of the confined/adsorbed phase in equilibrium with gas reservoir.

We have considered the H_2 molecules as spherical superatoms interacting via Lennard-Jones (6–12) potential. The quantum correction in the interaction model have included using the Feynman–Hibbs equations [13-15]. This correction makes the H_2-H_2 interaction energy slightly weaker with the effective intermolecular interaction slightly more repulsive. Additionally, the H_2-H_2 interaction parameters (ε = 34 K, σ = 2.96 nm) reported in [16] and largely applied in simulations of hydrogen adsorption in naporores [8-11] have been optimized to correctly reproduce bulk hydrogen density at 77 K reported in NIST data base. The optimized parameters (ε = 34 K, σ = 2.81 nm) were then applied in the present work.

The confining volume of nanometric size have been represented by simulation boxes of two different geometries. The first one, representing an infinite slit-shaped reservoir, consisted in parallelepiped of the lateral XY dimensions of 4.26 x 4.92 nm^2. The box dimension Z (Z = 1, 1.5, 2, 3, 4, and 5 nm) represented the distance H between the centers of the walls delimiting the reservoir. The second, tubular geometry was represented by the cylindrical box of the length of 4 nm and the diameter 2R = 1, 1.5, 2, 3, 4, or 5 nm. During simulations periodic boundary conditions (PBC) have been applied in the XY plane (along the cylinder' axis) for respectively slit-shaped (cylindrical) geometries (Fig.1a).

As we intend to simulate the gas *confined* but *not adsorbed* in the above described volumes, *there is no attraction* between hydrogen molecules and the reservoir' walls in our simulations. Such conditions were implemented and tested using three slightly different models of hydrogen-wall interaction: (i) the hard-wall type potential, assuming that the reservoir wall is built of carbon atoms, set to zero for hydrogen-wall distance greater than the sum of the H_2 and carbon atoms radii, otherwise being strongly repulsive (+∞), (ii) the soft-wall potential, assuming that the reservoir wall is built of non-attractive hydrogen molecules; we conserved the repulsive part of the potential, whereas the attractive part was set to zero, (iii) non-attractive carbon wall potential (NACW), assuming that the reservoir wall is built of non-attractive carbon atoms; again, we conserved the repulsive part of the potential, whereas the attractive part was set to zero (Figure 1b). The quantity of hydrogen (N_{gas}) confined in the simulation box was almost independent of the applied wall model (Fig1c). Therefore, we present here the results obtained using NACW interaction model only.

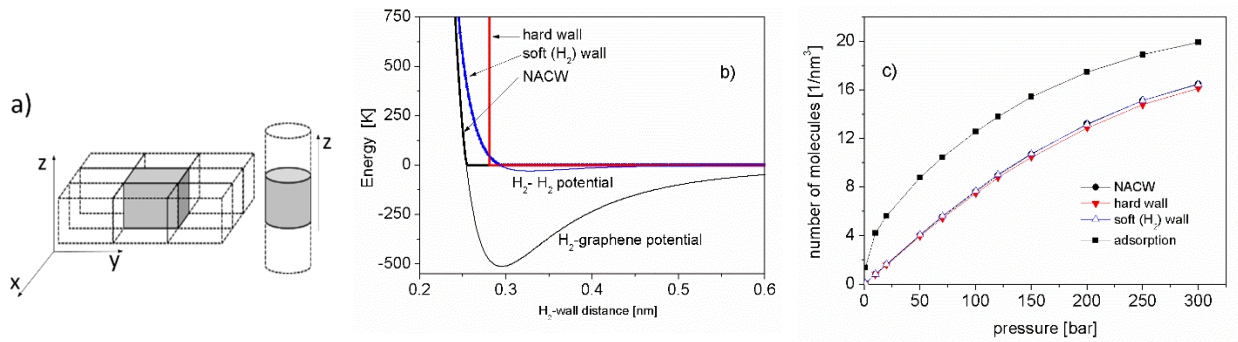

Figure 1. a) Implementation of PBC in slit-shaped and cylindrical geometry. The simulation boxes are shown in grey. The same coordinate system applies to both geometries. b) models of hydrogen-pore walls interactions. c) the number of hydrogen molecules confined in the simulation box, simulated using hard-wall, soft-wall, and non-attractive carbon wall (NACW) potentials, as a function of the external gas pressure. The box dimensions are 4.26 x 4.92 x 4.0 nm^3. For comparison, the number of molecules that can adsorb in slit-shaped carbon pore of the same dimensions is also shown.

3. Results and discussion

Figure 2 shows the average energy between hydrogen molecules confined in infinite slit-shaped and cylindrical *non-adsorbing* nanopores (nano-reservoirs), in a function of the reservoir size (width or diameter). For all pressure, the energy of interaction depends strongly on the pore size, in particular in micropore range (below 2 nm). In fact, as the interatomic energy is additive, its value depends on the local environment of molecules. For atoms located close to the pore walls the number of neighbors is reduced with respect to those located in the bulk; the contribution of these atoms to the average energy of the confined gas is small. When the size of a reservoir decreases, the fraction of such 'surface' atoms increases, and the average gas energy decreases. The effect is geometry-dependent and is more pronounced in cylindrical pores. In fact in slit geometry the local environment of the atoms close to the pore wall has more 2-dimensionnal (2D) character than for the atoms in the bulk (3D). These atoms are deprived of the neighbors in the direction perpendicular to the pore wall. In cylindrical pore this restriction is stronger, because of the pore wall curvature. In the limit of very small pore radius (R< 1 nm), only a single line of molecules can fit the cylindrical pore volume; the confinement is quasi 1-dimensional (1D), and the gas energy is the smallest. When the pore size increases, the difference between the energy of the gas confined in different geometries decreases also. It is the consequence of an increasing fraction of gas molecules having a 3D-type environment. For mesopores with pore sizes larger than 5 nm the contribution of molecules close to the pore walls becomes negligible and the average gas energy stabilizes at the value observed in the bulk gas.

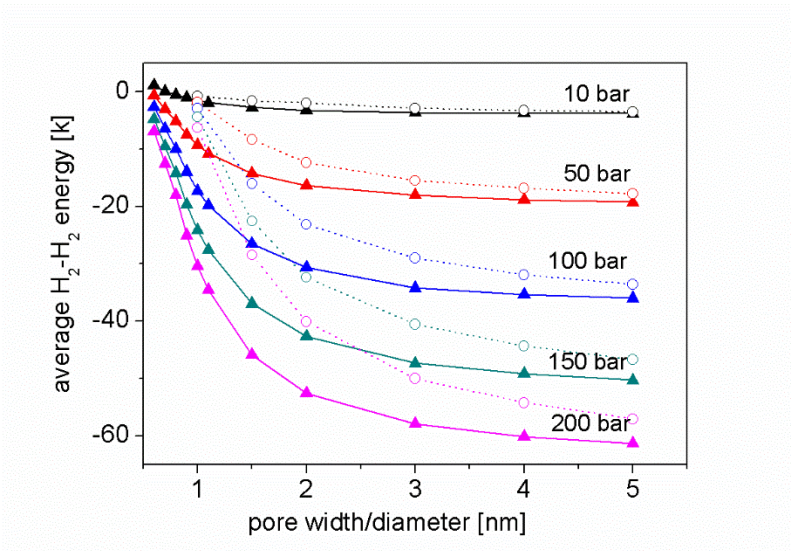

Figure 2. The average H_2-H_2 interaction energy at T=77 K as a function of the distance between the walls of infinite, slit shaped pore (closed triangles) or the diameter of an infinite cylindrical pore (open circles), for the applied external pressures of 10, 50, 100, 150, and 200 bars. The pore walls are non-attractive.

The observed variation of intermolecular energy with the pore size suggests that (i) the density of the gas in small pores must be lower than the bulk value, and (ii) the density must depend on the pore's size. This prediction, although intuitive, is physically easy to justify.

Figure 3 shows the distributions of hydrogen molecules confined in non-interacting slit shaped (middle panel) and cylindrical (right panel) pores of the size from 1 to 4 nm. For

comparison, the distribution of molecules in adsorbing pores is also shown (left panel). The heterogeneous

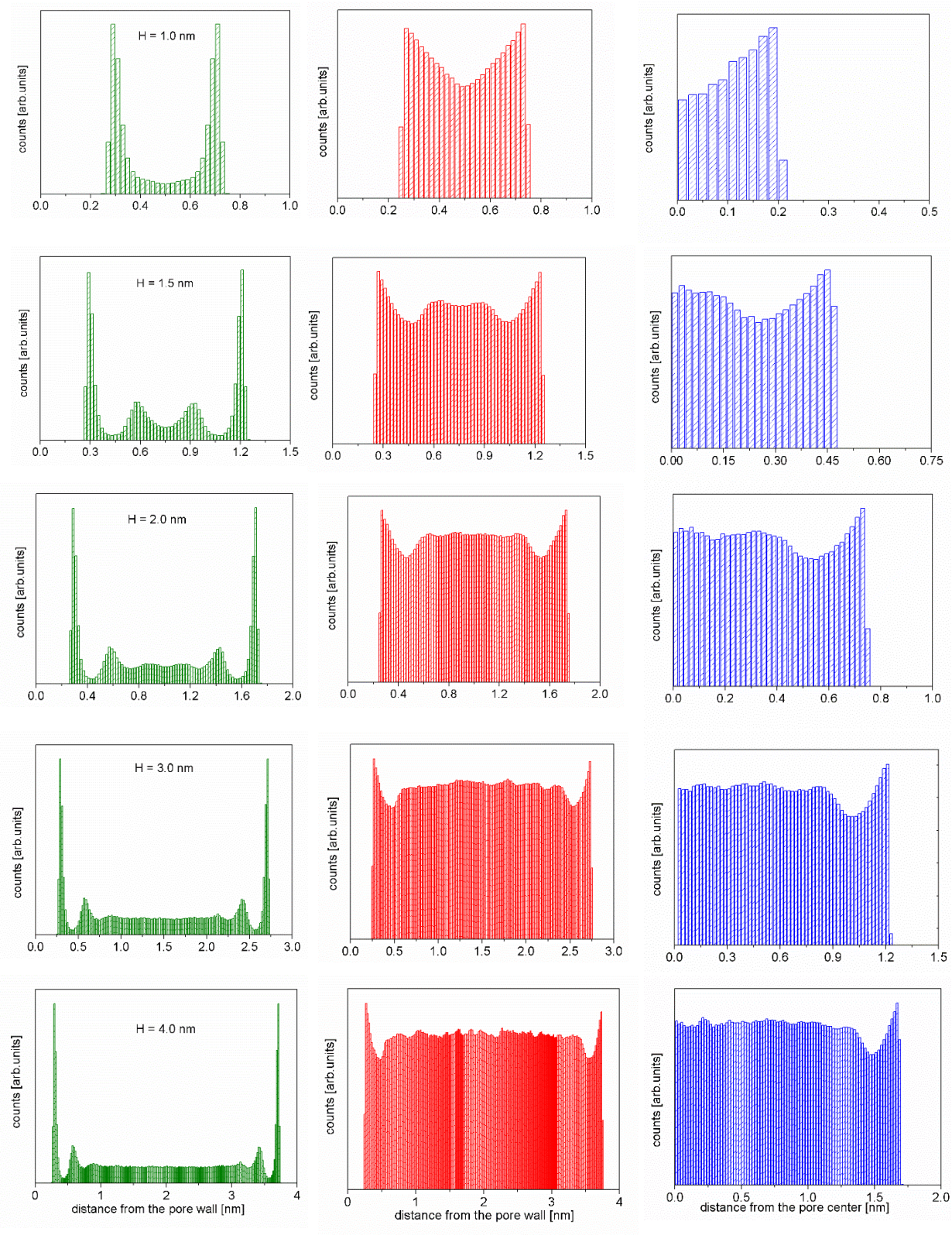

Figure 3. Distribution of density of hydrogen molecules *confined* in: (right column) - infinite cylindrical pores, (middle column) – infinite slit-shaped pores. For comparison, the distribution of molecules *adsorbed* in slit shaped pores is also shown (left column). T = 77

K. The vertical scales are different: the density of gas *adsorbed* in the middle of the pore is similar to the density of gas *confined* in non-adsorbing slit-pore.

distributions of adsorbed molecules (simulated using H_2-graphene potential shown in Fig.1c) is typical for low temperature adsorption of hydrogen [9,10]. The high concentration of molecules close to the pore wall results from hydrogen physisorption on graphene wall; the less intense second quasi-layer observed in larger pores, and the absence of further layers are the consequences of weak H_2-H_2 interaction. At the same time the gas distribution in non-adsorbing pores is also not uniform, and increases in the vicinity of the wall. The peak in distribution is observed even for the largest simulated pores. This behavior seems to be unintuitive, as for the 3D gas we expect a uniform distribution of molecules.

When the pore size increases above 2 nm, a plateau in the molecules distribution starts to develop at the pore center. Obviously, the density variation close to the pore walls will have negligible effect on the gas density in macroscopic volumes. However, when the pore size is smaller than 5nm, it will causes that the average density of the confined gas will be lower that its density in the bulk.

The macroscopic definition gives the density of a gas as the number of the particles (atoms or molecules) divided by the volume they occupy. When the density has to be evaluated from computer simulations, the number of particle is either known (because it is set constant as the input of simulations, i.e., in canonical ensemble) or constitute one of the main calculated results of simulations (i.e., $\langle N \rangle$ in grand canonical ensemble). On the other hand the gas volume, conventionally considered as the free space where the gas particles can be placed, requires a more precise definition if the gas is confined in porous structure. This definition is nothing but trivial if the confining structure is nanoporous.

The definition of accessible volume at nanoscale is not simple, and it is crucial for correct evaluation of the pore capacity. Figure 4a illustrates two possible approaches to define this volume. In the first one the accessible volume is simply defined as the pore volume physically occupied by the gas particles (total volume limited by the pore walls, stripped light grey area on Fig.4a). The second definition is formulated using the gas-wall interaction potential. In this approach the accessible volume is delimited by the coordinates where the interaction with pore wall becomes repulsive (Fig.1b). This volume corresponds to the space in the pore that is accessible to the centers of mass of particles, so obviously it is smaller than the total volume occupied by gas particles defined above. In the Fig. 4a it corresponds to the dark grey area in the middle of the pore.

The difference between these two volumes is negligible for macroscopic volumes. The reason is simple: the excluded volume is negligible in the macroscopic scale. However, at nanoscale, it introduces a large difference between the calculated averaged densities of the gas that can be confined in nanopores. This difference is never negligible for the pores of the size smaller than 5 nm. Figure 4b shows how the density in the slit pore depends on the definition of the pore size and the volume. The density is always calculated as the ratio between the number of particles and the accessible pore volume. A particle is included in the volume when its center of mass is located within the volume limits. The volume is defined as $V = S*(H - Z_{excluded})$. S is the surface of the slit pore wall. H is the pore size defined as the distance between the walls centers. $Z_{excluded} = 2*\Delta z$, where Δz is the distance between the wall center and the limit of particles' centers of mass distribution (see Fig.4a).

When the pore volume is defined as the whole space between the carbon walls ($Z_{excluded} = 0$, $V= S*H$), the gas density strongly depends on the pore size H. When the accessible pore

volume decreases ($0 < Z_{excluded} < 2*\Delta z$), the calculated density is increasing, as the number of particle within volume limits remains constant. For $Z_{excluded} > 2*\Delta z$ the calculated density will remain constant if the distribution of particles is homogeneous, or will slightly decrease/increase, depending on the particles' concentration close to the pore wall with respect to the pore interior. In both cases, the point of the slope change on the curves giving the calculated gas density vs. Δz marks the definition of the pore volume accessible for the gas. For hydrogen, as the concentration of molecules is higher in the vicinity of the pore wall (Fig.3, middle panel), the average density is decreasing for $Z_{excluded} > 2*\Delta z$. The $Z_{excluded}$ value for hydrogen confined in pores with non-interacting carbon wall is then estimated to be around $Z_{excluded} = 0.5$ nm.

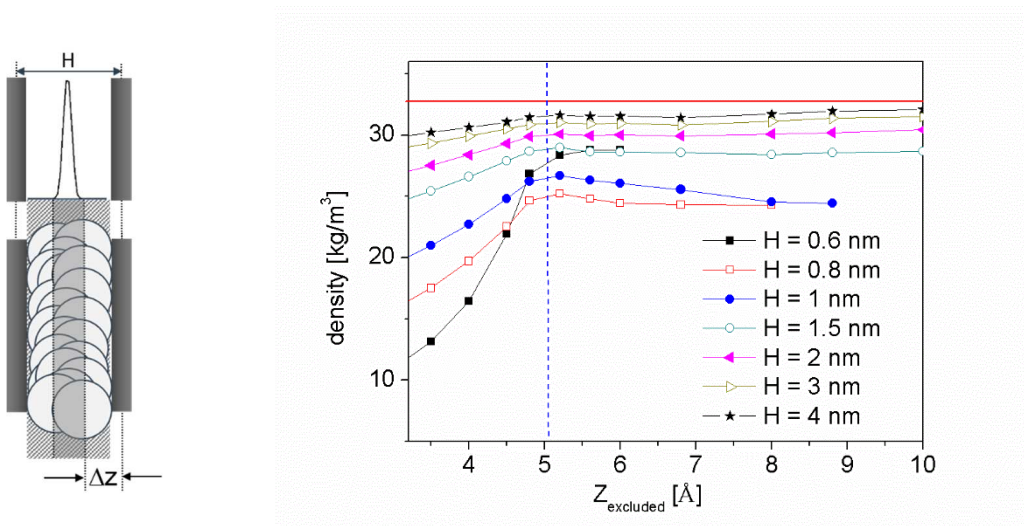

Figure 4. Left: model of a slit micropore of a size H. Stripped light grey: volume of the pore occupied by gas spherical particles. Dark grey: the volume (in the middle of the pore) accessible to the centers of mass of the gas particles. Black areas indicate the walls, not accessible to the particles. Right: gas apparent density as a function of the excluded distance $Z_{excluded} = 2*\Delta z$. The horizontal red line corresponds to the density ρ of the bulk hydrogen at 77 K: ρ = 32.81 g/l. The pressure of the bulk gas: 100 bar.

The excluded distance $Z_{excluded}$ determined above was then used to calculate the average density of hydrogen confined in non-adsorbing nanopores. Figure 5 shows the variation of this density with pressure, in slit-shaped (Fig.5a) and cylindrical (Fig.5b) nanopores of sizes H smaller than 5 nm. The mean densities are always smaller than the density of non-confined, 3D gas of hydrogen at the same pressures. For the moderate pressure of P = 100 bar, the relative difference between the bulk and confined gas densities is of the order of 12 % in the slit pore of the size H =1nm (22% in the cylindrical pore of the diameter of 1nm). This difference rapidly decreases when the pore size increases, and for slit of the width of H = 4 nm is only of the order of 2% (3% for cylindrical pore of the same diameter).

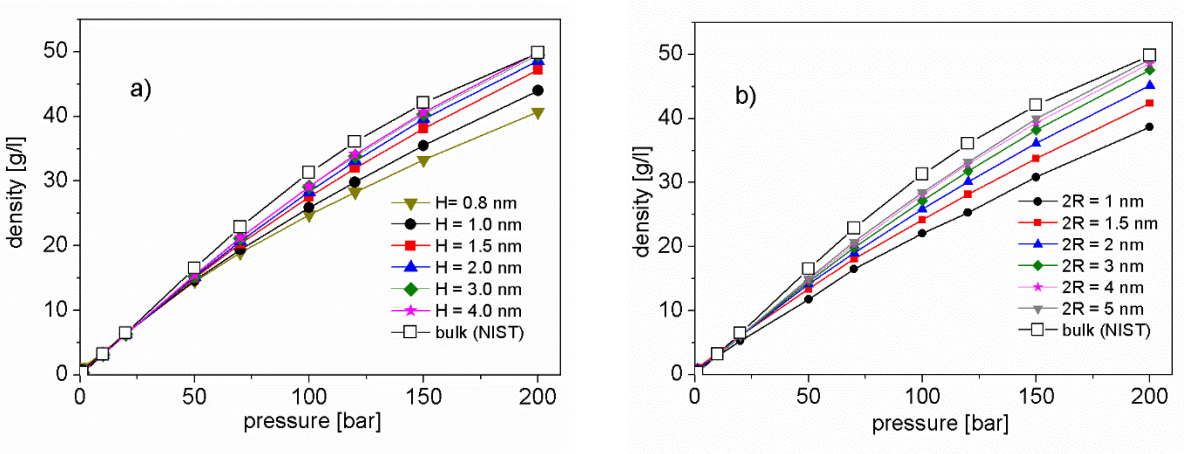

Figure 5. The average density of hydrogen confined at T=77 K in non-adsorbing a) infinite slit-shaped pore, b) infinite cylindrical pore, as a function of pressure. For comparison the density of bulk hydrogen [5] is also shown

Moreover, the distribution of the density is not homogeneous. As an example, Figure 6 shows the density distribution inside the slit shaped (cylindrical) pores of the width H (diameter) of 2 nm, for different pressures. At low pressures (P < 50 bar) the density is almost uniform within the pore volume, and its average value is within 5 % close to (although lower than) the bulk density. At the pressure P = 150 bar the gas density is visibly larger close to the pore wall. Further increase of pressure increases the heterogeneity of gas distribution. The molecules start to be closely packed on the pore wall. The density of this contact layer can be higher than the bulk density despite the lack of attraction from the pore walls. The effect of confinement is still noticeable beyond the contact layer, however, as the H_2-H_2 interaction is weak, no further structuration of the confined gas is observed up to P =200 bar. The density of the pore interior is homogeneous and smaller than bulk density.

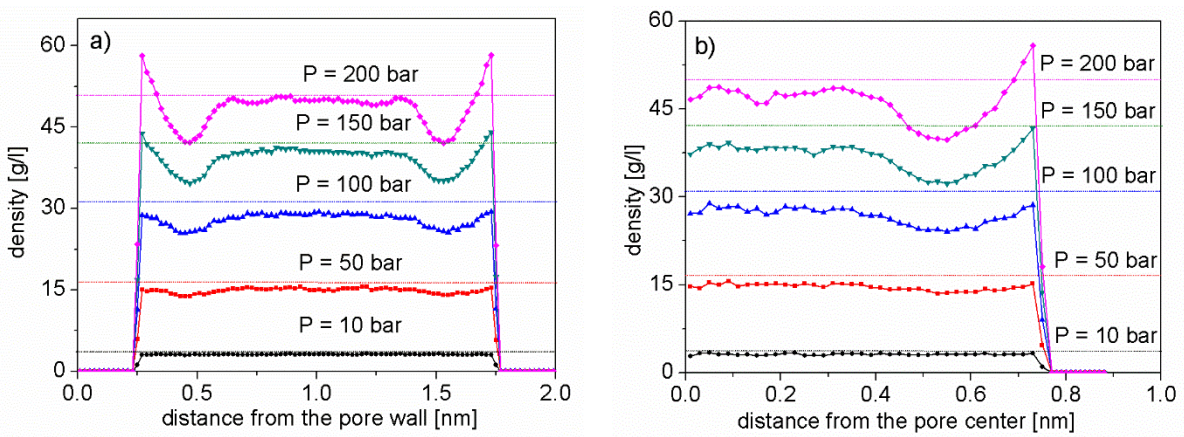

Figure 6. The distribution of density of hydrogen confined in non-attracting a) slit-shaped pore (pore width of 2 nm, b) cylindrical pore (pore diameter of 2 nm), for selected gas pressures. T = 77K. For comparison the density of bulk hydrogen [5] is also shown.

4. Conclusions

We have focused our study on the influence of confinement on properties of fluids, if the confining volumes are of nanometric size. Taking an example of hydrogen gas we have shown that the confined gas properties are different from their bulk analogs, even if the confining walls are non-attracting.

The most important difference consists in the observation that the density distribution inside the non-attracting reservoir is not homogeneous, and it strongly depends on the distance from the pore walls as well as on the pore size and on its shape. Such a behavior, although non-intuitive in macroscopic sample, has a simple physical explanation. The local energy of a given gas molecule strongly depends on the number of its nearest neighbors. In the nanopores this number decreases when the molecule-is closer to the pore wall.

Less intuitive is the observation that at higher pressures (p > 100 bar) the density of the gas close to the wall may be higher than in the middle of the pore. It can be even higher than the one of the bulk gas at the same thermodynamic conditions, despite weak H_2-H_2 interaction. This effect results from the geometric constrain of the molecules distribution close to the pore wall. The existence of non-attractive wall limits the translational fluctuations of the molecules which makes the average distance between molecules smaller and consequently the density higher.

We have observed similar heterogeneity of gas distribution in non-attractive nanopores also for other gases (Ar, Kr, N_2, CH_4, CO_2). However, because of the strong intermolecular interactions, these gases show slightly different density distribution close to the pore walls. We will analyze this behavior in a separate paper.

Our observations may affect some methodologies of adsorption measurements in nanoporous system with pores sizes below 5 nm. As the average density of the confined gas is smaller than the density of macroscopic gas quantity at the same thermodynamic conditions, the conversions of excess amount adsorbed into total amount using bulk gas density should be revisited.

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Declarations of interest: None.

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Figure Captions :

Figure 1. a) Implementation of PBC in slit-shaped and cylindrical geometry. The simulation boxes are shown in grey; b) models of hydrogen-pore walls interactions; c) the number of hydrogen molecules confined in the simulation box, simulated using hard-wall, soft-wall, and non-attractive carbon wall (NACW) potentials, as a function of the external gas pressure. The box dimensions are 4.26 x 4.92 x 4.0 nm^3. For comparison, the number of molecules than can adsorb in slit-shaped carbon pore of the same dimensions is also shown.

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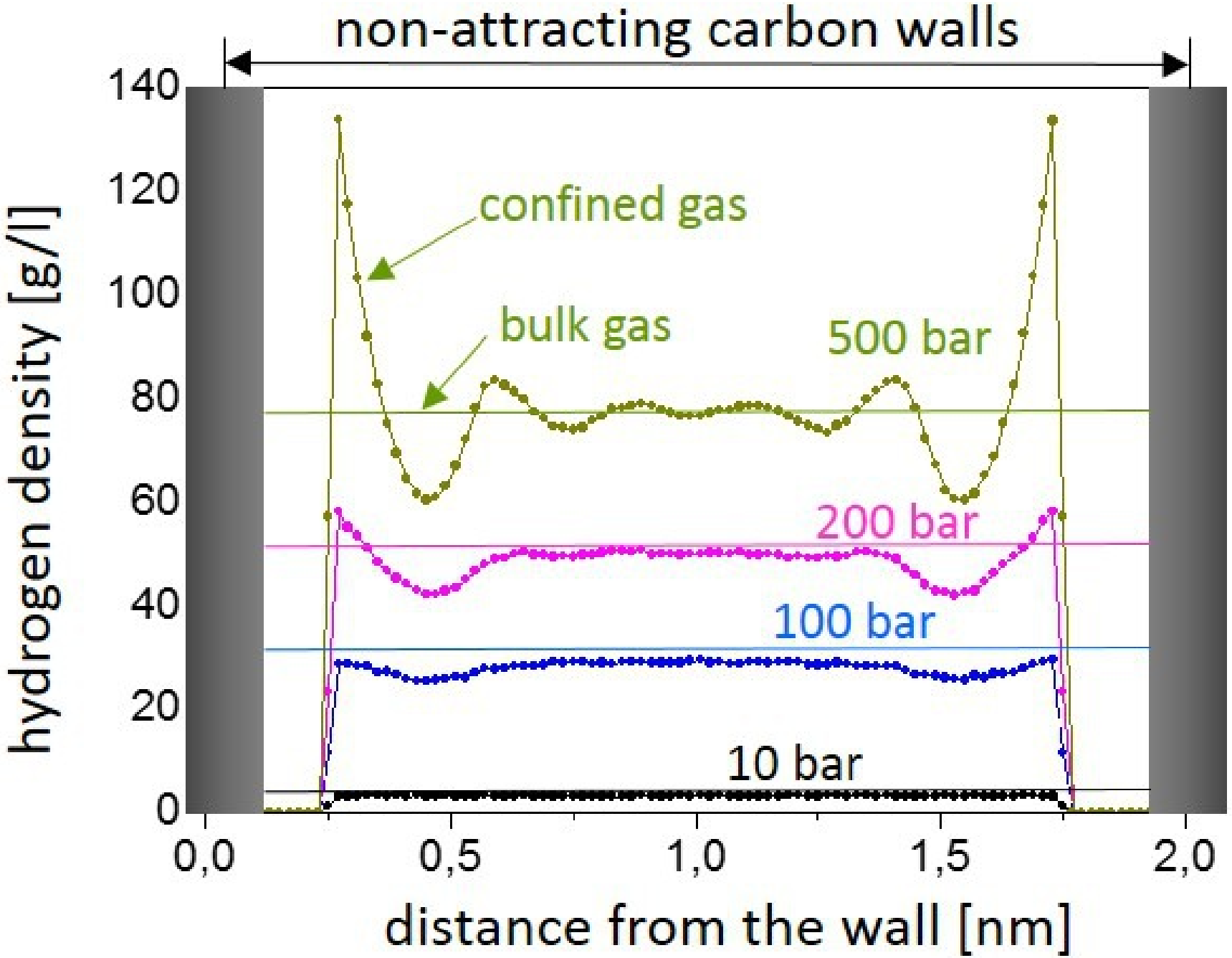
non-attracting carbon walls
confined gas
bulk gas
500 bar
200 bar
100 bar
10 bar
hydrogen density [g/l]
0
20
40
60
80
100
120
140
0,0
0,5
1,0
1,5
2,0
distance from the wall [nm]