

INTERNATIONAL SOCIETY FOR SOIL MECHANICS AND GEOTECHNICAL ENGINEERING



This paper was downloaded from the Online Library of the International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE). The library is available here:

<https://www.issmge.org/publications/online-library>

This is an open-access database that archives thousands of papers published under the Auspices of the ISSMGE and maintained by the Innovation and Development Committee of ISSMGE.

Use of nano-level constitutive model to predict the volume change behavior of the field expansive clay deposits

Sahel Abduljawwad

Civil & Environmental Engineering, KFUPM, Professor, Saudi Arabia, sajauwad@kfupm.edu.sa

Habib-ur-Rehman Ahmed

Civil & Environmental Engineering, KFUPM, Visiting Faculty, Saudi Arabia, habib.hurehman@gmail.com

ABSTRACT: Owing to their charged structures, clay minerals present in the subsurface soils adsorb moisture and are subjected to the volume change. This volume change induced by a change in moisture content poses problems for the stability of structures founded on these problematic soils. Because their overall behavior is controlled by the molecular level processes and interactions, a behavior model encompassing the contributions of these interactions is required to predict the behavior of the expansive clays consisting of a complex composition of clay and non-clay minerals exists. Authors developed a nano level constitutive model that incorporates all the major contributing factors such as moisture content, density, CEC, exchangeable cations, confining pressure, and interaction of clay minerals with non-clay minerals. As all the existing expansive clays constitutive models do not comprehensively incorporate all these factors, authors have used their developed nano level constitutive model for the natural expansive clays for the assessment of the volume change behavior of natural expansive clays in the field. The results were compared with the actual field studies on the volume change measurements of the expansive clay deposits in Qatif area of the Kingdom of Saudi Arabia.

RÉSUMÉ: En raison de leurs structures chargées, les minéraux argileux présents dans les sols souterrains adsorbent l'humidité ce qui entraîne un changement de leur volume. Cette variation en volume induite par le changement du niveau d'humidité peut avoir un impacte sur la stabilité des structures fondées sur ces sols instables. En raison du fait que leur comportement global est contrôlé par les processus et interactions à l'échelle moléculaire, un modèle englobant les contributions de ces interactions est nécessaire pour prédire le comportement des argiles expansives d'une composition complexe de minéraux argileux et non-argileux. Les auteurs ont pu développer un modèle constitutif qui intègre toutes les contributions des principaux facteurs à l'échelle nanométrique tels que le taux d'humidité, la densité, la CEC, les cations échangeables, la pression de confinement et l'interaction entre minéraux argileux et minéraux non-argileux. Les auteurs ont utilisé ce modèle afin d'évaluer le changement volumique des argiles expansives naturelles. Les résultats ont été comparés aux résultats d'études sur le terrain pour mesurer les changements volumiques des dépôts d'argile expansifs dans la région de Qatif du Royaume d'Arabie saoudite.

KEYWORDS: expansive clays; nano level behavior; constitutive modeling

1 INTRODUCTION

Expansive clays, whether natural or compacted, have a highly complex fabric and structure, with particles ranging in scale from nano-sized clay particles to sand- and/or silt-sized particles present in a random arrangement, with complex interactions among these particles. An understanding of the volume-change mechanism in expansive clay soils, therefore, requires the clear perception of the physicochemical interactions among the clay and non-clay particles at the molecular and/or nano levels, and of the coupling of the molecular level behavior at the macro level.

Because of their complexity, realistic numerical modeling of the volume-change behavior of expansive clays has been a long-standing challenge for geotechnical engineers. A realistic and representative constitutive model should encompass all of the factors such as moisture content, density, cation exchange capacity (CEC), interaction with other clay and non-clay minerals/particles, and their relative contributions to the physical, chemical and mechanical interactions at various scales. To integrate all of these factors into a constitutive model, understanding the behavior of the fabric at the molecular levels and linking it to the macroscopic behavior both in natural and in stabilized states is of fundamental importance.

Most of the existing models, however, pertain to the macro-levels only and do not incorporate the behavior prediction after potential chemical stabilization (Alonso et al. (1987), Alonso et al. (1990), Gens and Alonso (1992), Alonso et al. (1999), Sánchez et al. (2005), Guimaraes et al. (2013)) and only a few to the molecular level (Ichikawa et al. (2002), Karaborni et al.

(1996), Katti et al. (2005), Katti et al. (2009), Skipper (1992), Skipper et al. (1995a), Skipper et al. (1995b), Tao et al. (2010)).

We have formulated a comprehensive molecular-level model of expansive clay mineral fabric, encompassing all the earlier mentioned factors using molecular mechanics, molecular dynamics and Monte Carlo simulations (Ahmed and Abduljawwad, 2016). In this paper, we have validated this model for the assessment of the swell potential of the in-situ expansive clay deposits.

2 STUDY METHODOLOGY

The development of nanoscopic model constituted four major levels of activities; macro-level testing, micro-level imaging and analysis, molecular level simulation and modeling, and the formulation of a constitutive model. The fabric and structure of the natural and compacted soil samples, required as an input for the simulations, was evaluated using microscopic investigation and analysis through laboratory imaging techniques specified below, followed by the formulation of the constitutive model. The methodology of each level and the corresponding results are presented and discussed in the next sections while these are detailed in Ahmed and Abduljawwad (2016).

2.1 Macro-level tests

To compare the behavior of natural expansive-clay deposits and reconstituted laboratory specimens, we chose to use laboratory control specimens using various proportions of standard soil constituents. Therefore, in addition to obtaining undisturbed samples from natural expansive-soil deposits from Qatif and

Hofuf areas of Saudi Arabia, individual soil constituents were acquired from several known sources to serve as the control samples. To formulate the various combinations of known fabric and structure, control specimens with known proportions of clay minerals and non-clay minerals/particles were prepared with a variety of known densities and moisture contents. Swelling-potential tests were carried out on specimens prepared on the wet and dry side of optimum moisture content (OMC), following free swell test procedures in agreement with ASTM D4546 (Method A) and swelling pressure test under completely constrained conditions (Abduljawwad et al., 1998).

2.2 Microscopic investigations

Microscopic-level fabric testing and visualization of the pre- and post-swelling samples were carried out using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), micro-computed tomography (CT) scanning and environmental scanning electron microscopy (ESEM) using Rigaku Miniflex II, Micro-CT SkyScan 1172, Nicolet 6700 FTIR spectrometer, and FEI-Phillips ESEM-FEG Quanta 400 respectively at the Research Institute (RI) of KFUPM and R&D Center of Saudi Aramco at Dhahran, KSA.

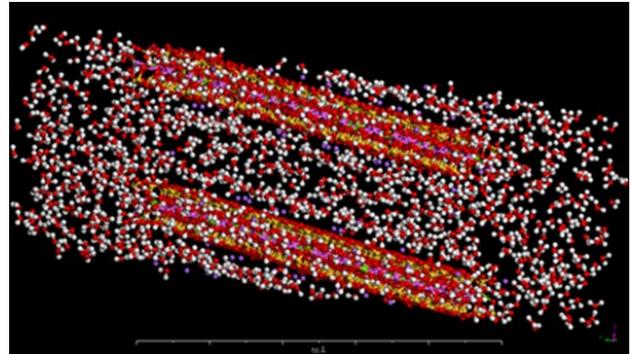
In addition to the mineralogical analysis, XRD data were also analyzed to determine the changes in d-spacing with moisture content and the assessment of the crystallite size using the Scherrer (1918) method. Using the Full Width at Half Maximum (FWHM) of the corresponding peaks in the XRD data after removal of background to obtain the net peak intensity have resulted in the assessment of the crystallite size in the range of 29 to 58 Å.

2.3 Molecular level modeling

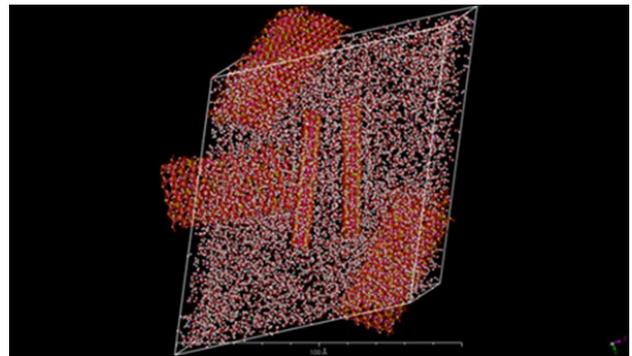
A molecular-level simulation was performed to study the processes and interactions occurring at the molecular level in the natural and compacted fabrics of the expansive soils. Any typical expansive clay soil consists of expansive clay minerals such as smectite, non-expansive clay minerals, such as kaolinite and illite, inert non-clay minerals such as quartz, and non-clay minerals interacting with expansive clay minerals such as calcite, gypsum, and other similar stabilizing salts. Cations and anions from these salts interact with expansive clay minerals and result in creating a cementation/induration effect on the clay minerals by changing the cohesion/adhesion among these particles. Non-clay mineral constituents such as quartz etc. only interact physically in the clay matrix. Therefore, in this study, the volume change processes are simulated using the clay mineral matrix and the associated salts while other non-clay minerals are considered not to change in volume. The overall volume change is therefore calculated based on the proportion of the clay minerals and associated salts in the soil matrix.

In this study, simulation techniques based on molecular mechanics (MM), molecular dynamics (MD) and Monte Carlo (MC) were used to study the interactions between clay and non-clay particles in the presence of various combinations of the interlayer and intralayer cations, anions and water under various fabric and structure conditions. The most important inputs for any molecular simulation scheme are the choice of the representative crystallites, formulation of the representative unit cells with periodic boundary conditions, and the application of a force field to run the appropriate ensemble. After the choice of the fundamental molecular size, the simulation was performed generally in seven steps (Figure 1): sorption of water molecules on the individual crystallites to create crystallites with different water contents, sorption and interaction of Na-montmorillonite crystallite with salts such as calcite, gypsum, and potassium chloride, assemblage of crystallites through natural randomness concepts in a periodic unit cell to create a soil fabric, compaction of the created fabric to the maximum

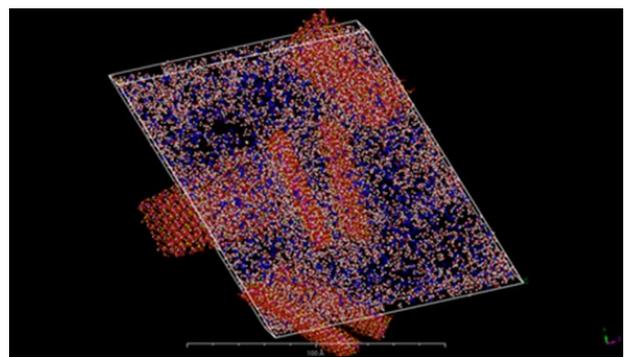
density, stress relaxation to simulate stress relief and, finally, volume change / swell and swell pressure assessment upon sorption of water molecules in the pore spaces. Simulations were carried out using Materials Studio software (2013) at the high-performance computing facilities (HPC) at KFUPM and the Supercomputing Laboratory (NESER) at the King Abdullah University of Sciences and Technology (KAUST).



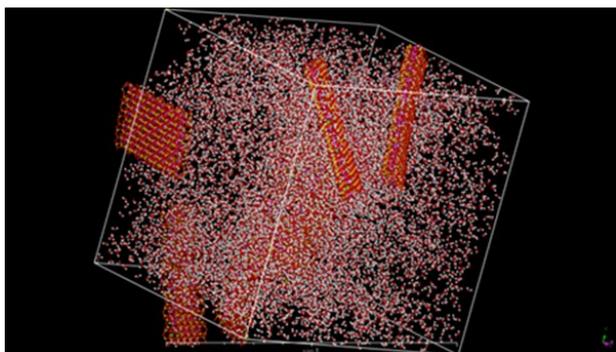
(a) Water sorption on single crystallite of Na-montmorillonite crystallite (water content = 60%) (Scale bar = 50 Å)



(b) Compaction of four crystallites of Na-montmorillonite in (a) to the maximum density at a confining pressure of 1 GPa (Scale bar = 100 Å)



(c) Water sorption in a stress relaxed unit cell (Scale bar = 100 Å)



(d) Unit cell after final volume change simulations (Scale bar = 150 Å)

Figure 1: Typical flow process of molecular simulations with all the stages from a) single crystallite b) compacted crystallites c) sorption of water molecules and d) final volume change of the periodic unit cell

3 NANOSCOPIC SWELL POTENTIAL CONSTITUTIVE MODEL

Using the results from the simulations and micro and macro testing, Ahmed and Abduljawad (2016) developed a nanoscopic swell potential constitutive model. In the development of this model, authors considered cohesive energy density (CED), moisture and density as three state parameters and the results of the molecular-level simulations of different CEC, moisture, density, exchangeable-cation and cementation effects under both free swell and swell pressure under the specified pressure boundary conditions were compiled to formulate a nanoscopic swell potential constitutive model. Quantitatively, CED is the amount of energy needed for the transition of a mol of material from the liquid to the gaseous phase and is considered as a measure of the mutual attractiveness of molecules. As CED concept is quite analogous to the processes controlling the volume change of swelling clays, it has been found to be sensitive to all the possible changes in the clay structure arising from variations in CEC, interlayer and intralayer-cations, anions, water, and density conditions. CED of the simulated loose mixes of the soil was determined by the Forcite module of the software. Using the relationship of CED to all these variables, a set of best-fit equations have been developed that collectively provide constitutive surfaces. A fundamental equation 1 relating the initial water content and the Total CED (TCED) is as follows.

$$TCED = 0.0625 (IWC)^3 - 3.575 (IWC)^2 + 10.5 (IWC) + 2830 + \Delta TCED_{CEC} + \Delta TCED_{cat} \quad (1)$$

TCED = total cohesive energy density in J/cm³, IWC = initial water content in percent, $\Delta TCED_{CEC}$ = correction due to CEC, $\Delta TCED_{cat}$ = correction due to binding / cementing salts and exchangeable cations

The fundamental TCED is then corrected for CEC, binding / cementing / stabilizing salts, and exchangeable cations using equations 2a, 2b, and 2c respectively developed from the change in CED due to all these factors.

$$\text{For } CEC > 90 \text{ meq/100 g} \\ \Delta TCED_{CEC} = [0.0717 (IWC)^3 - 3.775 (IWC)^2 - 22.917 (IWC) + 3785] (CEC - 90) / (144 - 90) \quad (2a)$$

$$\text{For } CEC < 90 \text{ meq/100 g} \\ \Delta TCED_{CEC} = [-0.0002 (IWC)^3 + 0.74 (IWC)^2 - 57.417 IWC + 1528] (90 - CEC) / (90 - 54) \quad (2b)$$

Equation 2 should be corrected for non-clay minerals / salts and the exchangeable cations as:

$$\Delta TCED_{cat} = [7100 (C/0.1) + 7250 (L/0.1) + 5050 (G/0.2) + 3010 (KCl/0.1) + 3250 (KP/0.1) + 3510 (D/0.1) + 10200 (P/0.1)] (10/IWC)^{0.85} + Ca(500) + Mg(300) + K(100) \quad (2c)$$

C = calcite, L = hydrated lime, G = gypsum, KCl = potassium chloride, KP = potassium phosphate, D = dolomite, P = palygorskite fraction of Na-Montmorillonite (Smectite) content & Ca = calcium exchangeable cation, Mg = magnesium exchangeable cation, K = potassium exchangeable cation fraction of the total cations

For CECs other than 54 meq/100g, equations 2 are normalized to equation 3.

$$TCED_m = e^{(0.01263 \times 54 + \ln(TCED) - 0.01263 CEC)} \quad (3)$$

Using TCED_m, final dry density (FDD) can be evaluated using equation 4.

$$FDD_I = [IDD + \{(0.000007 TCED_m + 0.3443) - IDD\}] (102/P)^{0.5} : TCED_m < 1610 \quad (4a)$$

$$FDD_{II} = [IDD + \{(0.0005 TCED_m - 0.4517) - IDD\}] (102/P)^{0.5} : TCED_m > 1610 \text{ and } < 3360 \quad (4b)$$

$$FDD_{III} = [IDD + \{(0.00006 TCED_m + 1.0082) - IDD\}] (102/P)^{0.5} : TCED_m > 3360 \quad (4c)$$

FDD is g/cm³, TCED_m in J/cm³, P = seating/confining pressure in kPa

The above equations result in 1-D swelling potential determined from the oedometer. As field swelling is 3-D in nature, following correction was applied to the 1-D swell from equations 1 to 4.

$$Swell_{field} = Swell_{lab} (Pa/Pc - 1) / 3 \quad (5)$$

Pa is applied pressure; Pc is preconsolidation pressure

Final water content at the terminal swell can be evaluated using the following relationship:

$$FWC_I = 0.0789 CED_{vw} + 56.648 (CED_{vw} < 87) \quad (6a)$$

$$FWC_{II} = 0.0039 (CED_{vw})^2 + 1.0587 CED_{vw} + 106.44 (CED_{vw} > 87) \quad (6b)$$

FWC = final water content in percent, IWC in percent, CED_{vw} in J/cm³

4 FIELD SWELLING ASSESSMENT USING NANOSCOPIC MODEL

The nanoscopic swell model was used to assess the swell of the in-situ natural expansive clays against author's comprehensive study (Abduljawad and Al-Sulaimani, 1993) to characterize and stabilize natural expansive clay soils from Qatif area of Saudi Arabia. In Abduljawad and Al-Sulaimani (1993), field plate load tests were performed on Al-Qatif expansive clay deposits. A 75 cm square plate was used to load a near surface 25 cm thick expansive clay layer with a surcharge pressure of 7 kPa. To simulate swell, water was added in a small channel dug around the plate assembly. The test was continued till no further heave of the plate was recorded. The characterization of the expansive clay layer is summarized in Table 1, while the swell versus time plot is shown in Figure 2.

Table 1: Properties of in-situ expansive soil (Abduljawwad and Al-Sulaimani (1993))

Parameters	Values and description
Natural water content (%)	40
Dry density, kN/m ³	1.1
Liquid limit (%)	150
Plastic limit (%)	55
X-ray results	Smectite (52%), Illite (23%), palygorskite (5%), dolomite (9%), gypsum (6%), and quartz (5%)
CEC (meq/100 g)	57

The model developed by Ahmed and Abduljawwad (2106) was used to predict the swell percent for the three different stabilizers at various percentages. Using the CEC, mineralogical composition, initial moisture content, and density as the input in equations 1 to 5, the swell percent was calculated for a 25 cm thick expansive clay layer. Water content at the final swell state was assessed from equation 6. Variation of the swell on the water content was then plotted in Figure 2. Figure 2 shows a comparison between the swell percent from the field test value and the one predicted by the nanoscopic swell model. It could be noted from the comparison in Figure 2 that the results predicted by the model are very close to the experimental value. Moreover, the variations in volume change versus intake water content match very closely to the variations of actual field swell against time.

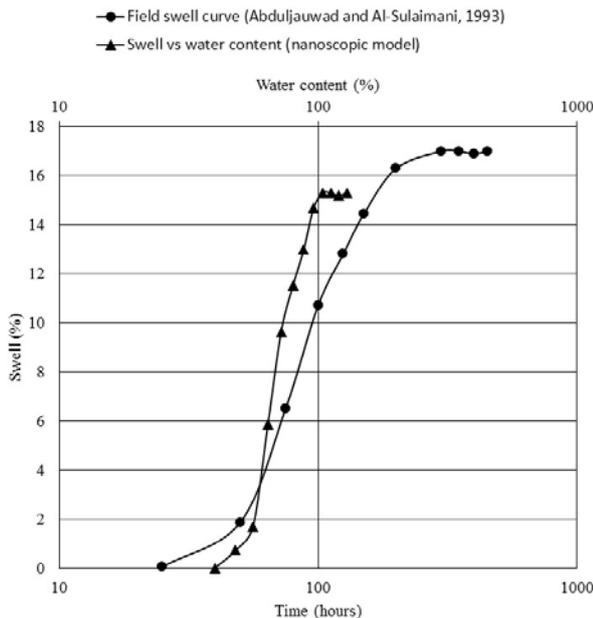


Figure 2. Comparison of the field swell vs. time curve (Abduljawwad and Al-Sulaimani, 1993) with the predicted swell vs. water content curve by the nanoscopic model.

5 CONCLUSIONS

The nanoscopic swell model has been developed to elucidate the behavior of expansive clay soils encompassing the variation in CEC, moisture content, density, and complex interactions between clay and non-clay minerals, salts, and stabilizers.

The nanoscopic model, together with the provided parameters and procedures, has been successfully applied for the assessment of swell/volume change of the in-situ expansive

clay deposits. It has also provided quite close predictions of the variations of the volume change with intake water content.

6 ACKNOWLEDGEMENTS

Authors would like to acknowledge King Fahd University of Petroleum & Minerals (KFUPM) for the highly valuable support throughout this research.

7 REFERENCES

- Abduljawwad S.N. and Al-Sulaimani G.J. (1993). Determination of swell potential of Al-Qatif Clay. *Geotechnical Testing Journal*, 16(4):469–484.
- Abduljawwad S.N., Al-Sulaimani G.J., Basunbul I.A., and Al-Buraim I. (1998). Laboratory and field studies of the response of structures to heave of expansive clay. *Geotechnique* 48(1):103–121.
- Ahmed H.R. and Abduljawwad S.N. (2016). Nano-level constitutive model for expansive clays”. *Geotechnique*, DOI, [http://dx.doi.org/10.1680/jgeot.15.P.140], 2016.
- Alonso E.E., Gens A. and Hight D.W. (1987). Special Problem Soils, General Report. In a *Proceedings 9th European Conference on Soil Mechanics*, Dublin, 3, pp 1087–1146.
- Alonso E.E., Gens A. and Josa A. (1990). A constitutive model for partially saturated soils. *Geotechnique*, 40(3):405–430.
- Alonso E.E., Vaunat J. and Gens A. (1999). Modeling the mechanical behavior of expansive Clays. *Engineering Geology* 54:173–83.
- ASTM (2014) D4546: Standard Test Methods for One-Dimensional Swell or Collapse of Soils. ASTM International, West Conshohocken, PA, USA.
- Clay Minerals Society (2013) Source Clays Physical / Chemical Data. <http://www.clays.org/SOURCE%20CLAYS/SCdata.html>.
- Gens A. and Alonso E.E. (1992). A framework for the behavior of unsaturated expansive clays. *Canadian Geotechnical Journal* 29:1013–1032.
- Guimarães L., Gens A., Sánchez M. and Olivella S. (2013) A chemo-mechanical constitutive model accounting for cation exchange in expansive clays. *Geotechnique* 63(3): 221–234.
- Hameed R.A. (1991) Characterization of Expansive Soils in the Eastern Province of Saudi Arabia. MS Thesis, KFUPM, Dhahran, Saudi Arabia.
- Ichikawa Y., Kawamura K., Fuji N. and Nattavut T. (2002). Molecular dynamics and multiscale homogenization analysis of seepage-diffusion problem in bentonite clay. *International Journal of Numerical Methods in Engineering* 54:1717–1749.
- Karaborni S., Smit B., Heidug W., Urai E. and van Oort (1996). The Swelling of Clays: Molecular Simulations of the Hydration of Montmorillonite. *Science* 271:10–15.
- Katti D.R., Schmidt S., Ghosh P. and Katti K.S. (2005). Modeling Response of Pyrophyllite Clay Interlayer to Applied Stress Using Steered Molecular Dynamics. *Clays and Clay Minerals* 52(2):171–178.
- Katti D.R., Matar M.I., Katti K.S. and Amarasinghe P.M. (2009). Multiscale Modeling of Swelling Clays: A Computational and Experimental Approach. *KSCCE Journal of Civil Engineering* 13(4):243–255.
- Materials Studio v7.0 (2013), Accelrys Software Inc., US.
- Sánchez M., Gens A., Guimarães L.N. and Olivella S. (2005). A double structure generalized plasticity model for expansive materials. *International Journal for Numerical and Analytical Methods in Geomechanics* 29:751–787.
- Scherrer P. (1918). Bestimmung der Größe und der inneren Struktur von Kolloidteilchen mittels Röntgenstrahlen. *Nachr. Ges. Wiss. Göttingen* 26:98–100.
- Skipper N.T., Sposito G. and Chang F.R. (1995a). Monte Carlo simulations of interlayer molecular structure in swelling clay minerals I. Methodology. *Clays and Clay Minerals* 43(3):285–293.
- Skipper N.T., Sposito G. and Chang F.R. (1995b). Monte Carlo simulations of interlayer molecular structure in swelling clay minerals I. Monolayer Hydrates. *Clays and Clay Minerals* 43(3):294–303.
- Tao L., Xiao-Feng T., Yu Z. and Tao G. (2010). Swelling of K⁺, Na⁺ and Ca²⁺ - montmorillonites and hydration of interlayer cations: a molecular dynamics simulation. *Chin. Phys. B* 19(10):50-55.