

## Responses to the comments of Reviewer #2:

C1. *The authors claim that they added "quasi two-dimensional molecular crystals" in lines 9-10. Unfortunately, they write "geometry" instead of "crystals" what is not satisfactory! The same description should be included also in the Significance Statement.*

R1. We are sorry for the contradiction. We have corrected the lines 9-10 of the abstract to "quasi two-dimensional molecular crystals". In the Significant Statement, we have revised lines 7-8 as "We construct a molecular model of two-dimensional crystals", and remove "We find that" in line 9 to fit within 120 words.

C2. *In the resubmission, the authors disclose their MD procedure; they explain that molecular melting occurs at much high temperatures that transitions related to molecular orientation. What is missing is that they should earlier in the text describe that their model system has two kind of transitions: high temperature transition between liquid and hexagonal crystal (with no orientational order) and at low temperatures transitions between various orientational orderings including liquid, hexatic, and crystalline skyrmions. Here they focus to low temperature orientational ordering.*

R2. We agree we need to explain in the main text that the two-dimensional crystalline state is stable in the temperature range we study. We have added in lines 80-86 "There are two-step phase transitions between liquids, orientationally disordered crystals, and orientationally ordered crystals shown in Fig. 1. The melting temperature is much higher than that of the orientational phase transition. In the present study we focus on low-temperature range, wherein the two-dimensional hexagonal crystal is stable (see Materials and Methods for the detail).".

C3. *It would be good to replay also to my question about torques. Their MD approach include toques only in the basic dynamic equations. As the authors in the text mention also effects of external fields and similarities to cholesterics it would be good explain if a description based on a torque exhibited by an external field on the director used for liquid crystals can be applied also here.*

R3. Yes, it is possible to apply continuum description to find the ground state molecular orientation under external fields, though it is difficult to find the direct correspondence with the Landau-de Gennes free energy concerning molecular field. In lines 416-425 we have added "The molecular torque is given by  $\partial U / \partial \mathbf{n}_i$ . From Eq.8, the ground state of molecular orientation is given by  $\sum_j (\vec{1} - \mathbf{n}_i \mathbf{n}_i) \cdot (\partial U / \partial \mathbf{n}_i) = \chi_a (\mathbf{n}_i \cdot \mathbf{H}) (\mathbf{H} - (\mathbf{n}_i \cdot \mathbf{H}) \mathbf{n}_i)$ , where  $U_{ij}$  is the first term in Eq.1, representing intermolecular interaction. This equation indicates the balance between the molecular field (the l.h.s.) and the torque arising from the external field (the r.h.s.), where the stable root of the latter is  $\mathbf{n} \parallel \mathbf{H}$  ( $\mathbf{n} \perp \mathbf{H}$ ) for  $\chi_a >$

**0** ( $\chi_a < 0$ ), consistent with the continuum description in liquid crystals (1). Thus, in Fig.4B and C, molecular orientation aligns parallel and perpendicular to strong external fields, respectively.”. We have also added “(see Materials and Methods, Eq.(8) and the following sentences).” in lines 241-242 in the main text.