Effect of a built-in field in asymmetric ferroelectric tunnel junctions

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From last presentation:

Magic Happens…

- Very opaque to me
- Hooke’s law-like terms
- Polarization-dependence
- Some cross-terms?
- Why?
- Who knows?

$$\tilde{\mathcal{F}} = \mathcal{F} + \eta_1\sigma_1 + \eta_2\sigma_2 + \eta_6\sigma_6 \quad (76)$$

must be performed in order to study the equilibrium properties of this constrained film.

For pedagogical simplicity, we consider a uniaxial ferroelectric where P is the polarization in the z-direction. The free energy, with condition (74), of a cubic ferroelectric is [48]

$$\mathcal{F} = \mathcal{F}_P - \boxed{\frac{1}{2}s_{11}(\sigma_1^2 + \sigma_2^2)} - \boxed{Q_{12}\{(\sigma_1 + \sigma_2)P^2\}} - \boxed{s_{12}\sigma_1\sigma_2 - \frac{1}{2}s_{44}\sigma_6^2} \quad (77)$$

where Q_{ij} and s_{ij} are the electrostrictive constants and the elastic compliances at constant polarization respectively. Using $\frac{\partial \mathcal{F}}{\partial \sigma_i} = -\eta_i$, and solving for $\sigma_1 = \sigma_2 = \bar{\sigma}$ (in this special case $\sigma_6 = 0$), we find that

$$\boxed{\tilde{\mathcal{F}} = \frac{\bar{\eta}^2}{s_{11} + s_{12}} + \frac{1}{2}\tilde{a}P^2 + \frac{1}{4}\tilde{b}P^4 + \frac{1}{6}cP^6} \quad (78)$$

where

$$\tilde{a} = a - \frac{4\bar{\eta}Q_{12}}{s_{11} + s_{12}} \quad (79)$$

and

$$\tilde{b} = b + \frac{4Q_{12}^2}{s_{11} + s_{12}} \quad (80)$$

The resolution!:

- Do a Legendre transform (like getting Hamiltonain from Lagrangian in CM or thermodynamics)
  - Solve $\frac{\partial \mathcal{F}}{\partial \sigma_i} = -\eta_i$ and substitute back to get expression in terms of σ_i.

- Math offered as appendix to presentation

Reminder:

(i) Bulk free energy
(ii) Depolarization energy
(iii) Build-in field due to electrodes
(iv) Surface energy

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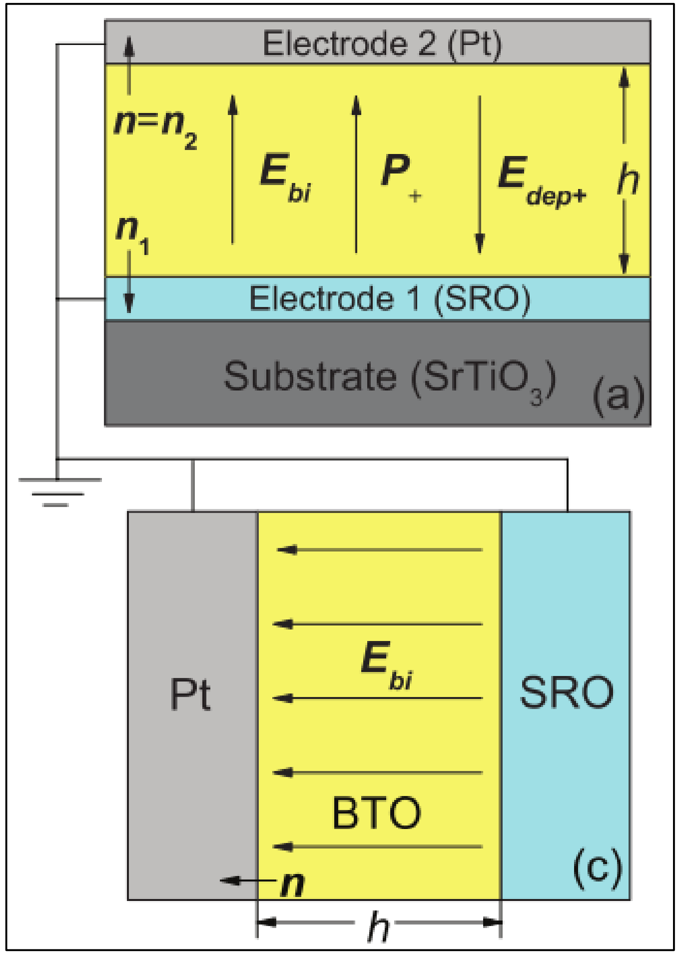
Effect of a built-in electric field in asymmetric ferroelectric tunnel junctions

Yang Liu,[1,2,*] Xiaojie Lou,[1] Manuel Bibes,[3] and Brahim Dkhil[2]

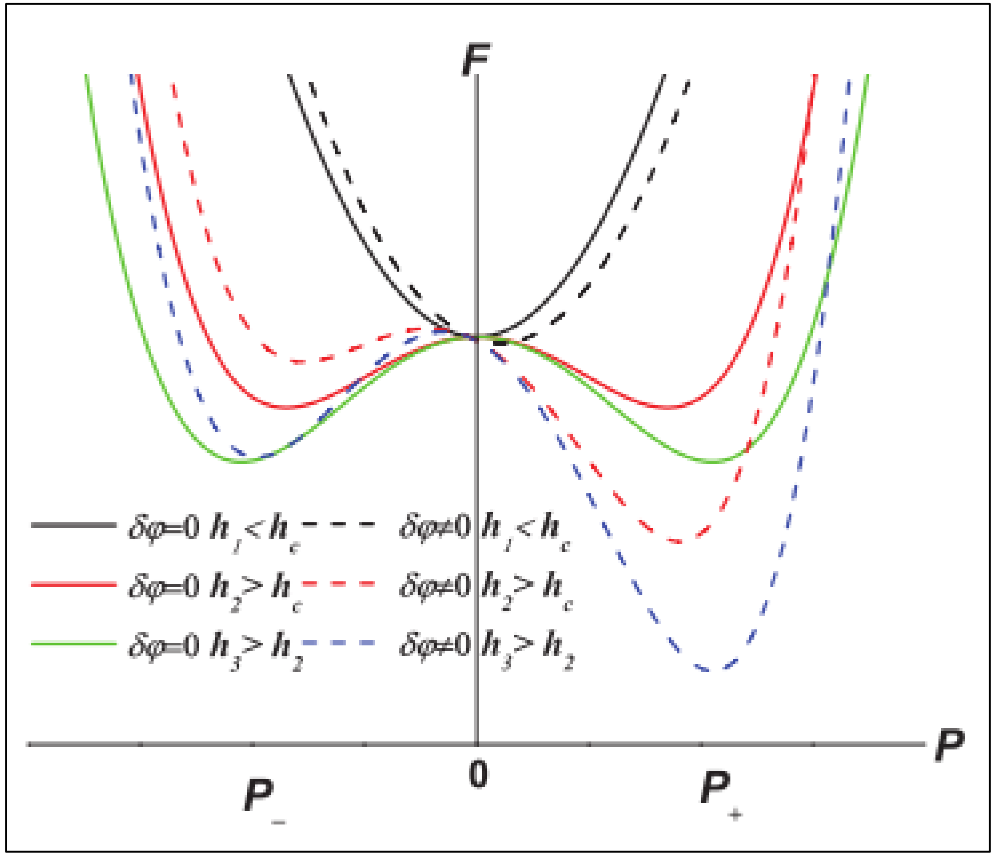
$$\begin{aligned} F = h\Phi + \boxed{\Phi_S} = \Bigg(& \boxed{\frac{1}{2}\alpha_1^* P^2 + \frac{1}{4}\alpha_{11}^* P^4 + \frac{1}{6}\alpha_{111} P^6} \\ & \boxed{+ \frac{1}{8}\alpha_{1111} P^8 + \frac{u_m^2}{S_{11} + S_{12}}} - \boxed{\frac{1}{2}\vec{E}_{\text{dep}} \cdot \vec{P}} \boxed{- \vec{E}_{bi} \cdot \vec{P}} \\ & \boxed{- \vec{E} \cdot \vec{P} \Bigg) h} + \boxed{(\zeta_1 - \zeta_2)\vec{n} \cdot \vec{P} + \frac{1}{2}(\eta_1 + \eta_2) P^2}, \end{aligned}$$

System considered:

- STO(001)/SRO/BTO/Pt, fully strained
- Consider $\eta_1 = \eta_2, \zeta_1 = \zeta_2$ to simplify (*slightly*)
  - $F = \left(\frac{1}{2}\alpha_1^* P^2 + \frac{1}{4}\alpha_{11}^* P^4 + \frac{1}{6}\alpha_{111} P^6 + \frac{1}{8}\alpha_{1111} P^8 + \frac{u_m^2}{S_{11}+S_{12}} - \frac{1}{2}\vec{E}_{dep} \cdot \vec{P} - \vec{E}_{bi} \cdot \vec{P}\right) h + \eta P^2$
  - $\vec{E}_{bi} = -\frac{\delta\varphi}{h}\vec{n}$
- Leads to a familiar picture…



Free energy vs. P:

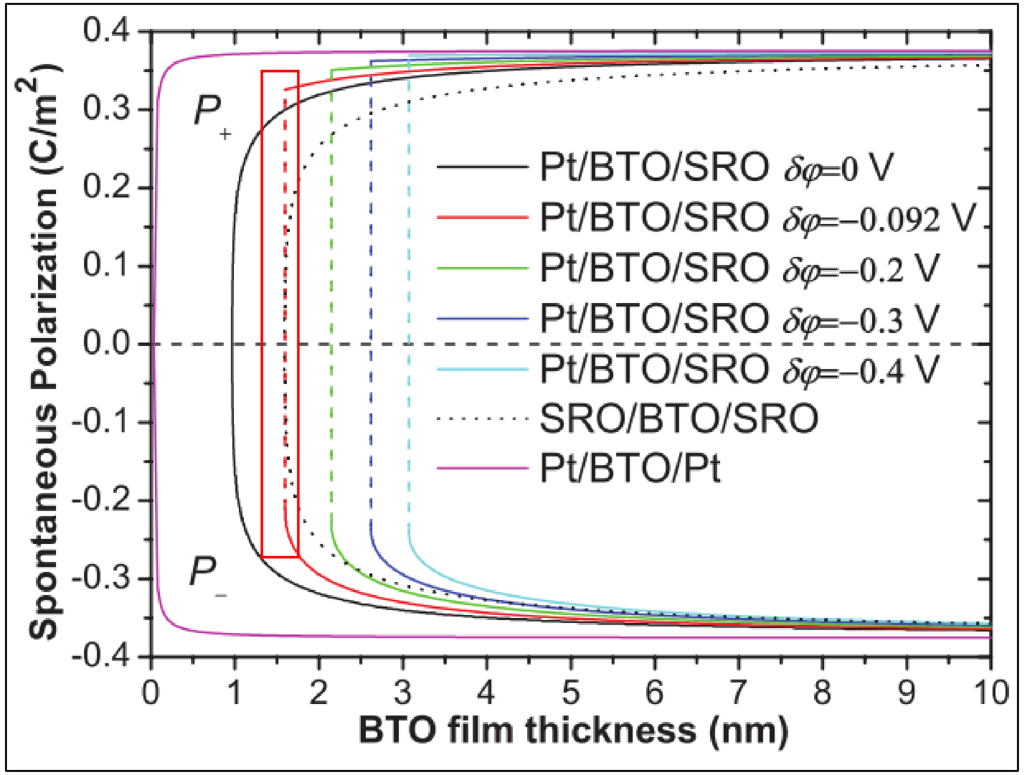


- Above h_c, BTO has two stable minima & one unstable
  - $\delta\varphi \neq 0$ tilts F vs. P profile

- Below h_c, one minima
  - $\delta\varphi \neq 0$ gives stable, nonzero, nonswitchable polarization
  - “Polar non-FE” phase proposed in paper

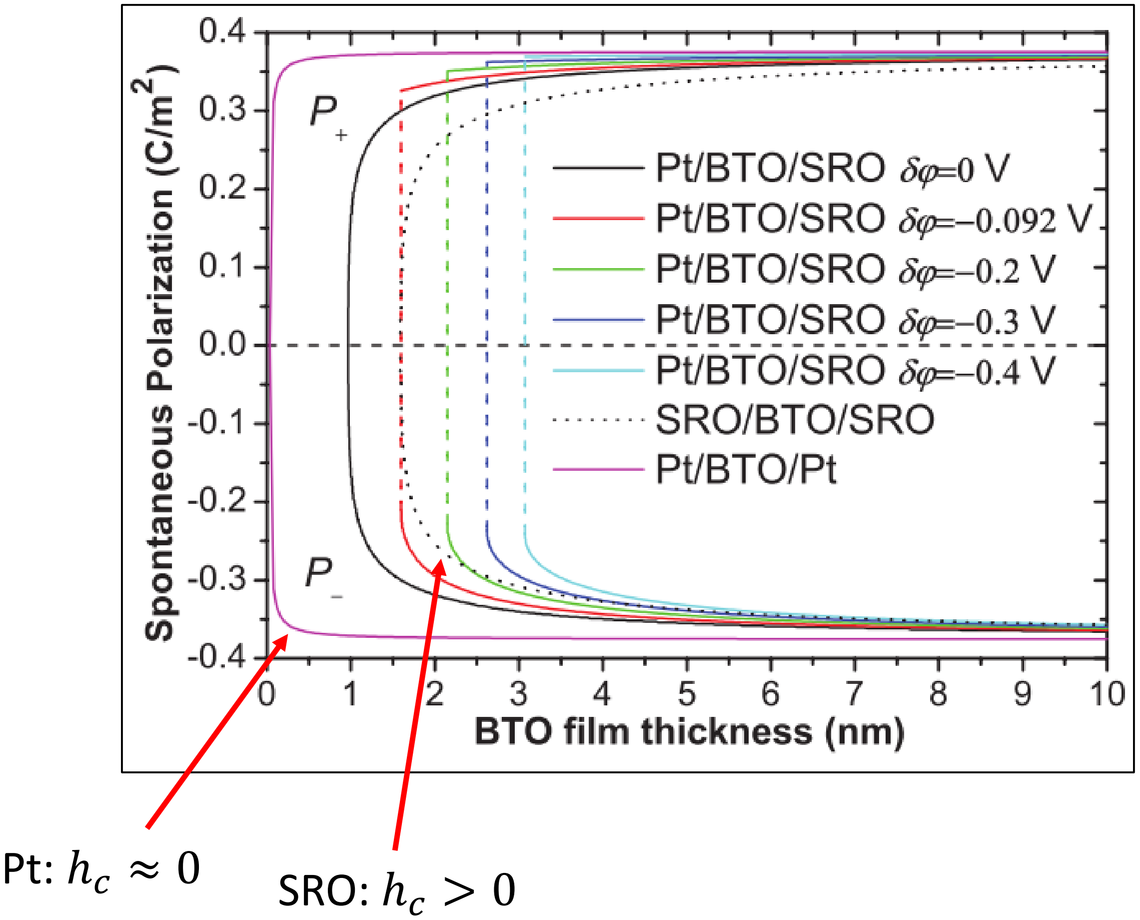
Main result:

- Shifting of hysteresis ($|P_+| \neq |P_-|$)
- General increase of h_c with increased built-in field
- Asymmetric curves of P_+, P_- near h_c

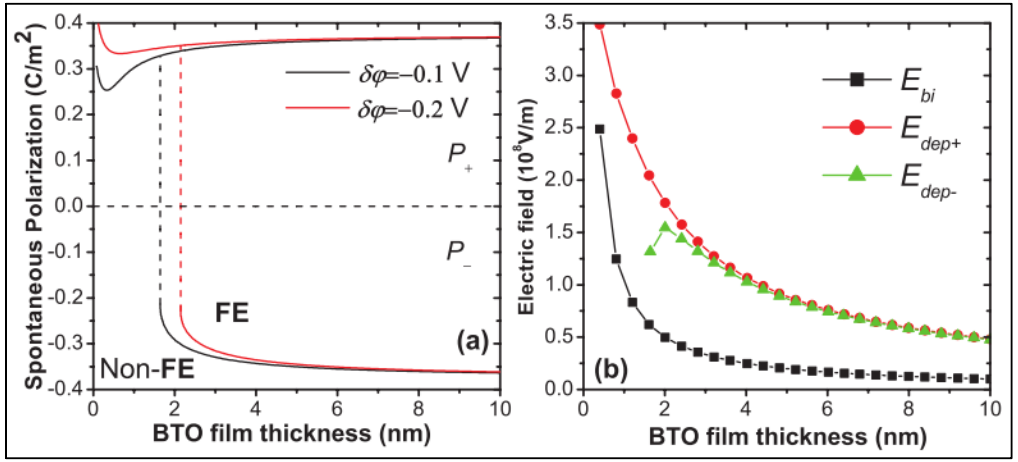


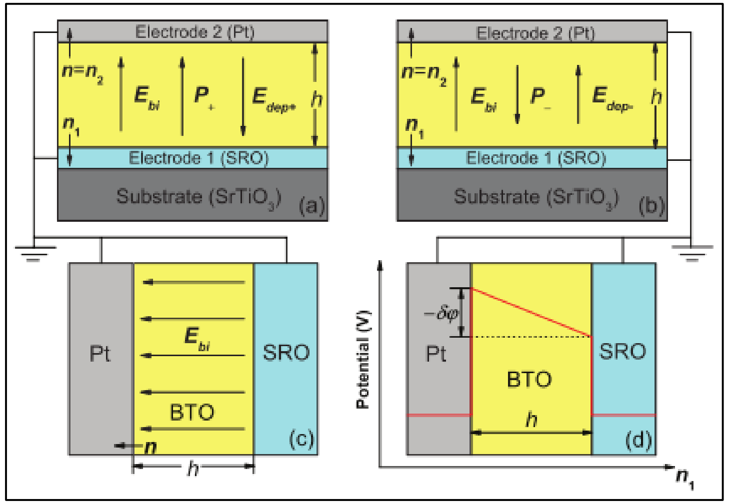
SRO/BTO/SRO & Pt/BTO/Pt:

- Question: why do these symmetric structures look so different?
- Thought 1: $u_m = 0$ for Pt structures
- Thought 2: Difference in screen length gives different $\vec{E}_{dep}$



Origin of non-FE polarization:

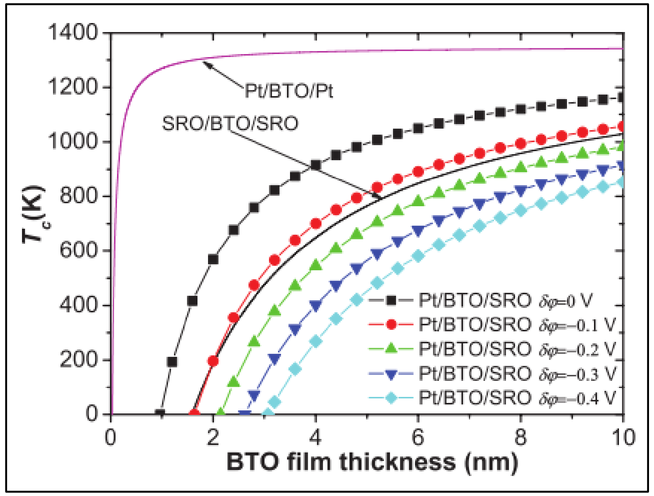


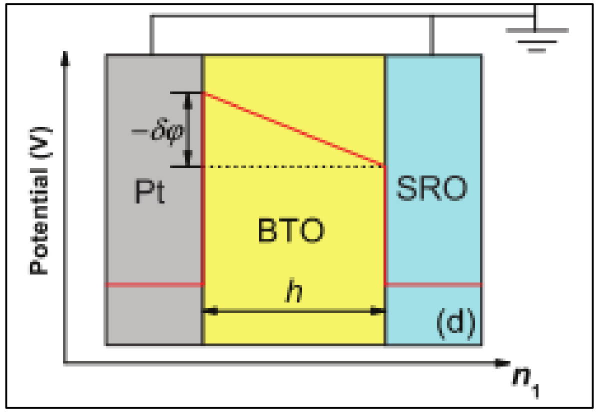


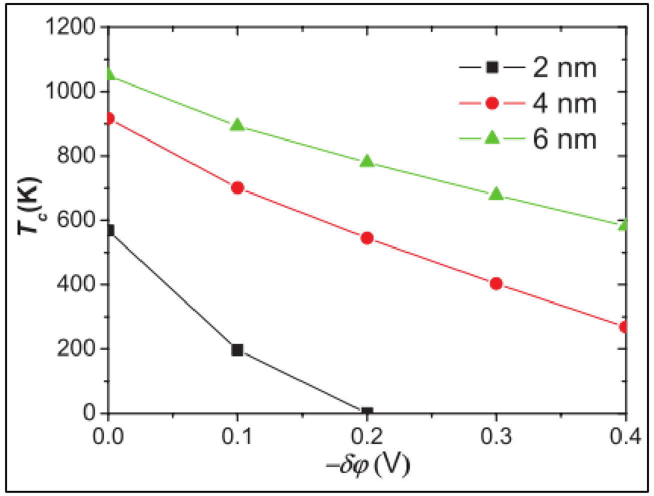
- Single domain FE states are stable even at low thickness
- Domains form to minimize electrostatic energy
  - However, 180˚ stripe domains are unfavorable
- Paper: non-switchable domains form to minimize energy

TER effect still present:

- Asymmetry in built-in potential leads to TER observed
- Switching of $\delta\varphi$ or addition of interfacial asymmetry $\zeta_1 \neq \zeta_2$ keeps main results
- Transition temperature more sensitive in thinner FEs
  - Electrocaloric effect: Should take into account sources of heating







Thanks!

Mathematical appendix

$$\frac{\partial \mathcal{F}}{\partial \sigma_1} = -\eta_1 \Rightarrow \eta_1 = -\left[-S_{11}\sigma_1 - Q_{12}P^2 - S_{12}\sigma_2\right]$$

Let $\bar{\eta} = S_{11}\bar{\sigma} + Q_{12}P^2 + S_{12}\bar{\sigma} = Q_{12}P^2 + (S_{11}+S_{12})\bar{\sigma}$

$$\Rightarrow \boxed{\bar{\sigma} = \frac{\bar{\eta} - Q_{12}P^2}{S_{11}+S_{12}}}$$

$$\tilde{\mathcal{F}} = \mathcal{F} + 2\bar{\sigma}\bar{\eta} = \mathcal{F} + \frac{2\bar{\eta}^2 - 2Q_{12}\bar{\eta}P^2}{S_{11}+S_{12}}$$

$$\tilde{\mathcal{F}} = \mathcal{F}_P - \tfrac{1}{2}S_{11}(2\bar{\sigma}^2) - Q_{12}2\bar{\sigma}P^2 - S_{12}\bar{\sigma}^2 + \frac{2\bar{\eta}^2}{S_{11}+S_{12}} - \frac{2Q_{12}\bar{\eta}P^2}{S_{11}+S_{12}}$$

$$= \mathcal{F}_P - S_{11}\left[\frac{\bar{\eta}-Q_{12}P^2}{S_{11}+S_{12}}\right]^2 - 2Q_{12}P^2\left[\frac{\bar{\eta}-Q_{12}P^2}{S_{11}+S_{12}}\right] - S_{12}\left[\frac{\bar{\eta}-Q_{12}P^2}{S_{11}+S_{12}}\right]^2 + \frac{2\bar{\eta}^2}{S_{11}+S_{12}} - \frac{2Q_{12}\bar{\eta}P^2}{S_{11}+S_{12}}$$

$$= \mathcal{F}_P - \frac{S_{11}}{(S_{11}+S_{12})^2}\left[\bar{\eta}^2 - 2\bar{\eta}Q_{12}P^2 + Q_{12}^2P^4\right] - \frac{2Q_{12}P^2}{(S_{11}+S_{12})}\left[\bar{\eta} - Q_{12}P^2\right] - \frac{S_{12}}{(S_{11}+S_{12})^2}\left[\bar{\eta}^2 - 2Q_{12}\bar{\eta}P^2 + Q_{12}^2P^4\right]$$

$$+ \frac{2\bar{\eta}^2}{S_{11}+S_{12}} - \frac{2Q_{12}\bar{\eta}P^2}{S_{11}+S_{12}}$$

$$\tilde{\mathcal{F}} = \mathcal{F}_P - \left[\frac{S_{11}}{(S_{11}+S_{12})^2}\bar{\eta}^2 + \frac{S_{12}}{(S_{11}+S_{12})^2}\bar{\eta}^2\right] + \left[\frac{S_{11}}{(S_{11}+S_{12})^2}\cdot 2\bar{\eta}Q_{12} - \frac{2Q_{12}\bar{\eta}}{(S_{11}+S_{12})} + \frac{2Q_{12}\bar{\eta}S_{12}}{(S_{11}+S_{12})^2}\right]P^2$$

$$+ \left[\frac{-S_{11}}{(S_{11}+S_{12})^2}Q_{12}^2 + \frac{2Q_{12}^2}{(S_{11}+S_{12})} - \frac{S_{12}Q_{12}^2}{(S_{11}+S_{12})^2}\right]P^4 + \frac{2\bar{\eta}^2}{(S_{11}+S_{12})} - \frac{2Q_{12}\bar{\eta}P^2}{(S_{11}+S_{12})}$$

$$= \mathcal{F}_P + \left[\frac{2\bar{\eta}^2}{S_{11}+S_{12}} - \frac{(S_{11}+S_{12})\bar{\eta}^2}{(S_{11}+S_{12})^2}\right] + \left[\frac{2Q_{12}S_{11}\bar{\eta}}{(S_{11}+S_{12})^2} - \frac{4Q_{12}\bar{\eta}}{(S_{11}+S_{12})} + \frac{2Q_{12}S_{12}\bar{\eta}}{(S_{11}+S_{12})^2}\right]P^2$$

$$+ \left[\frac{2Q_{12}^2}{S_{11}+S_{12}} - \frac{(S_{11}+S_{12})Q_{12}^2}{(S_{11}+S_{12})^2}\right]P^4$$

$$= \mathcal{F}_P + \frac{\bar{\eta}^2}{S_{11}+S_{12}} + \frac{2Q_{12}\bar{\eta}(S_{11}+S_{12})}{(S_{11}+S_{12})^2}P^2 - \frac{4Q_{12}\bar{\eta}}{(S_{11}+S_{12})}P^2 + \frac{2Q_{12}^2 - Q_{12}^2}{(S_{11}+S_{12})}P^4$$

$$= \mathcal{F}_P + \frac{\bar{\eta}^2}{S_{11}+S_{12}} - \frac{2Q_{12}\bar{\eta}}{(S_{11}+S_{12})}P^2 + \frac{Q_{12}^2}{(S_{11}+S_{12})}P^4$$

$$= \frac{1}{2}\left(a - \frac{4Q_{12}\bar{\eta}}{S_{11}+S_{12}}\right)P^2 + \frac{1}{4}\left(b + \frac{4Q_{12}^2}{S_{11}+S_{12}}\right)P^4 + \frac{1}{6}cP^6 + \frac{\bar{\eta}^2}{S_{11}+S_{12}}$$